Unit 2: Linear models: Inference

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We now understand the least squares estimator $\hat{\beta}$ from geometric and algebraic points of view. In Unit 2, we will switch to a probabilistic perspective to derive inferential statements for linear models, in the form of hypothesis tests and confidence intervals. In order to facilitate this, we will assume that the error terms are normally distributed:

$$y = X\beta + \epsilon$$
, where $\epsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$. (1)

1 Building blocks for linear model inference

First we put in place some building blocks: The multivariate normal distribution (Section 1.1), the distributions of linear regression estimates and residuals (Section 1.2), and estimation of the noise variance σ^2 (Section 1.3).

1.1 The multivariate normal distribution

Recall that a random vector $w \in \mathbb{R}^d$ has a multivariate normal distribution with mean μ and covariate matrix Σ if it has probability density

$$p(\boldsymbol{w}) = \frac{1}{\sqrt{(2\pi)^d \text{det}(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\boldsymbol{w} - \boldsymbol{\mu})^T \Sigma^{-1}(\boldsymbol{w} - \boldsymbol{\mu})\right).$$

These random vectors have lots of special properties, including:

- (Linear transformation) If $w \sim N(\mu, \Sigma)$, then $Aw + b \sim N(A\mu + b, A\Sigma A^T)$.
- (Independence) If $\begin{pmatrix} \boldsymbol{w}_1 \\ \boldsymbol{w}_2 \end{pmatrix} \sim N \begin{pmatrix} \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{pmatrix} \end{pmatrix}$, then $\boldsymbol{w}_1 \perp \!\!\! \perp \boldsymbol{w}_2$ if and only if $\boldsymbol{\Sigma}_{12} = \boldsymbol{0}$.

An important distribution related to the multivariate normal is the χ_d^2 (chi-squared with d degrees of freedom) distribution, defined as

$$\chi_d^2 \equiv \sum_{j=1}^d w_j^2$$
 for $w_1, \dots, w_d \stackrel{\text{i.i.d.}}{\sim} N(0, 1)$.

1.2 The distributions of linear regression estimates and residuals

The most important distributional result in linear regression is that

$$\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T \boldsymbol{X})^{-1}).$$
 (2)

Indeed, by the linear transformation property of the multivariate normal distribution,

$$\boldsymbol{y} \sim N(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 \boldsymbol{I}_n) \Longrightarrow \widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y} \sim N((\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{X}\boldsymbol{\beta}, (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \sigma^2 \boldsymbol{I}_n \boldsymbol{X} (\boldsymbol{X}^T \boldsymbol{X})^{-1})$$
$$= N(\boldsymbol{\beta}, \sigma^2 (\boldsymbol{X}^T \boldsymbol{X})^{-1}).$$

Next, let's consider the joint distribution of $\hat{\mu} = X\hat{\beta}$ and $\hat{\epsilon} = y - X\hat{\beta}$. We have

$$\begin{pmatrix}
\widehat{\boldsymbol{\mu}} \\
\widehat{\boldsymbol{\epsilon}}
\end{pmatrix} = \begin{pmatrix}
\boldsymbol{H} \boldsymbol{y} \\
(\boldsymbol{I} - \boldsymbol{H}) \boldsymbol{y}
\end{pmatrix} = \begin{pmatrix}
\boldsymbol{H} \\
\boldsymbol{I} - \boldsymbol{H}
\end{pmatrix} \boldsymbol{y} \sim N \begin{pmatrix} \begin{pmatrix} \boldsymbol{H} \\ \boldsymbol{I} - \boldsymbol{H} \end{pmatrix} \boldsymbol{X} \boldsymbol{\beta}, \begin{pmatrix} \boldsymbol{H} \\ \boldsymbol{I} - \boldsymbol{H} \end{pmatrix} \cdot \sigma^2 \boldsymbol{I} \begin{pmatrix} \boldsymbol{H} & \boldsymbol{I} - \boldsymbol{H} \end{pmatrix} \\
= N \begin{pmatrix} \begin{pmatrix} \boldsymbol{X} \boldsymbol{\beta} \\ \boldsymbol{0} \end{pmatrix}, \begin{pmatrix} \sigma^2 \boldsymbol{H} & \boldsymbol{0} \\ \boldsymbol{0} & \sigma^2 (\boldsymbol{I} - \boldsymbol{H}) \end{pmatrix} \end{pmatrix}. \tag{3}$$

In other words,

$$\widehat{\boldsymbol{\mu}} \sim N(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 \boldsymbol{H}) \quad \text{and} \quad \widehat{\boldsymbol{\epsilon}} \sim N(\boldsymbol{0}, \sigma^2 (\boldsymbol{I} - \boldsymbol{H})), \quad \text{with} \quad \widehat{\boldsymbol{\mu}} \perp \perp \widehat{\boldsymbol{\epsilon}}.$$
 (4)

Since $\hat{\beta}$ is a deterministic function of $\hat{\mu}$ (in particular, $\hat{\beta} = (X^T X)^{-1} X^T \hat{\mu}$), it also follows that

$$\hat{\boldsymbol{\beta}} \perp \!\!\!\perp \hat{\boldsymbol{\epsilon}}.$$
 (5)

1.3 Estimation of the noise variance σ^2

We can't quite do inference for β based on the distributional result (2) because the noise variance σ^2 is unknown to us. Intuitively, since $\sigma^2 = \mathbb{E}[\epsilon_i^2]$, we can get an estimate of σ^2 by looking at the quantity $\|\hat{\epsilon}\|^2$. To get the distribution of this quantity, we need the following lemma:

Lemma 1.1. Let $\mathbf{w} \sim N(\mathbf{0}, \mathbf{P})$ for some projection matrix \mathbf{P} . Then, $\|\mathbf{w}\|^2 \sim \chi_d^2$, where $d = \operatorname{trace}(\mathbf{P})$ is the dimension of the subspace onto which \mathbf{P} projects.

Proof. Let $P = UDU^T$ be an eigenvalue decomposition of P, where U is orthogonal and D is a diagonal matrix with $D_{ii} \in \{0,1\}$. We have $\mathbf{w} \stackrel{d}{=} UD\mathbf{z}$ for $\mathbf{z} \sim N(0, \mathbf{I}_n)$. Therefore,

$$\|\boldsymbol{w}\|^2 = \|\boldsymbol{D}\boldsymbol{z}\|^2 = \sum_{i:D_{ii}=1} z_i^2 \sim \chi_d^2$$
, where $d = |\{i:D_{ii}=1\}| = \operatorname{trace}(D) = \operatorname{trace}(P)$.

Recall that I - H is a projection onto the (n - p)-dimensional space $C(X)^{\perp}$, so by Lemma 1.1 and equation (4) we have

$$\|\widehat{\boldsymbol{\epsilon}}\|^2 \sim \sigma^2 \chi_{n-p}^2. \tag{6}$$

From this result, it follows that $\mathbb{E}[\|\hat{\epsilon}\|^2] = n - p$, so

$$\widehat{\sigma}^2 \equiv \frac{1}{n-p} \|\widehat{\boldsymbol{\epsilon}}\|^2 \tag{7}$$

is an unbiased estimate for σ^2 . Why does the denominator need to be n-p rather than n for the estimator above to be unbiased? The reason for this is that the residuals $\hat{\epsilon}$ are the projection of the true noise vector ϵ onto the lower-dimensional subspace $C(X)^{\perp}$. To see this, note that

$$\widehat{\boldsymbol{\epsilon}} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y} = (\boldsymbol{I} - \boldsymbol{H})(\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}) = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{\epsilon}. \tag{8}$$

2 Hypothesis testing

Typically two types of null hypotheses are tested in a regression setting: Those involving onedimensional parameters and those involving multi-dimensional parameters. For example, consider the null hypotheses $H_0: \beta_j = 0$ and $H_0: \beta_S = \mathbf{0}$ for $S \subseteq \{0, 1, ..., p-1\}$, respectively. We discuss tests of these two kinds of hypothesis in Sections 2.1 and 2.2, and then discuss the power of these tests in Section 2.3.

2.1 Testing a one-dimensional parameter

t-test for a single coefficient. The most common question to ask in a linear regression context is: Is the jth predictor associated with the response, when controlling for the other predictors? In the language of hypothesis testing, this corresponds to the null hypothesis

$$H_0: \beta_i = 0. (9)$$

According to (2), we have $\hat{\beta}_j \sim N(0, \sigma^2/s_j^2)$, where, as we learned in Unit 1,

$$s_j^2 \equiv [(\boldsymbol{X}^T \boldsymbol{X})_{jj}^{-1}]^{-1} = \|\boldsymbol{x}_{*j}^{\perp}\|^2. \tag{10}$$

Therefore,

$$\frac{\widehat{\beta}_j}{\sigma/s_j} \sim N(0,1),\tag{11}$$

and we are tempted to define a level α test of the null hypothesis (9) based on this normal distribution. While this is infeasible since we don't know σ^2 , we can substitute in the unbiased estimate (7) derived in Section 1.3. Then,

$$SE_j \equiv \frac{\widehat{\sigma}}{s_j}$$
 is the standard error of $\widehat{\beta}_j$, (12)

which is an approximation to the standard deviation of $\hat{\beta}_j$. Dividing $\hat{\beta}_j$ by its standard error gives us the t-statistic

$$t_j \equiv \frac{\widehat{\beta}_j}{\mathrm{SE}_j} = \frac{\widehat{\beta}_j}{\sqrt{\frac{1}{n-p} \|\widehat{\epsilon}\|^2 / s_j}}.$$
 (13)

This statistic is *pivotal*, in the sense that it has the same distribution for any β such that $\beta_j = 0$. Indeed, we can rewrite it as

$$t_j = \frac{\frac{\widehat{\beta}}{\sigma/s_j}}{\sqrt{\frac{\sigma^{-2}\|\widehat{\mathbf{e}}\|^2}{n-p}}}.$$
 (14)

Recalling the independence of $\widehat{\beta}$ and $\widehat{\epsilon}$ (5), the scaled chi square distribution of $\|\widehat{\epsilon}\|^2$ (6), the standard normal distribution of $\frac{\widehat{\beta}}{\sigma/s_i}$ (11), we find that

under
$$H_0: \beta_j = 0$$
, $t_j \sim \frac{N(0,1)}{\sqrt{\frac{1}{n-p}\chi_{n-p}^2}}$, with numerator and denominator independent. (15)

The latter distribution is called the t distribution with n-p degrees of freedom and denoted t_{n-p} . This paves the way for the two-sided t-test:

$$\phi_t(\mathbf{X}, \mathbf{y}) = \mathbb{1}(|t_j| > t_{n-p}(1 - \alpha/2)),$$
(16)

where $t_{n-p}(1-\alpha/2)$ denotes the $1-\alpha/2$ quantile of t_{n-p} . Note that, by the law of large numbers,

$$\frac{1}{n-p}\chi_{n-p}^2 \stackrel{P}{\to} 1 \quad \text{as} \quad n-p \to \infty, \tag{17}$$

so for large n-p we have $t_j \sim t_{n-p} \approx N(0,1)$. Hence, the t-test is approximately equal to the following z-test:

$$\phi_t(\boldsymbol{X}, \boldsymbol{y}) \approx \phi_z(\boldsymbol{X}, \boldsymbol{y}) \equiv \mathbb{1}(|t_i| > z(1 - \alpha/2)), \tag{18}$$

where $z(1 - \alpha/2)$ is the $1 - \alpha/2$ quantile of N(0, 1). The t-test can also be defined in a one-sided fashion, if power against one-sided alternatives is desired.

Example: One-sample model. Consider the intercept-only linear regression model $y = \beta_0 + \epsilon$, and let's apply the t-test derived above to test the null hypothesis $H_0: \beta_0 = 0$. We have $\hat{\beta}_0 = \bar{y}$. Furthermore, we have

$$SE_0^2 = \frac{\hat{\sigma}^2}{n}, \quad \text{where} \quad \hat{\sigma}^2 = \frac{1}{n-1} \| \boldsymbol{y} - \bar{y} \boldsymbol{1}_n \|^2.$$
 (19)

Hence, we obtain the t statistic

$$t = \frac{\widehat{\beta}_0}{\mathrm{SE}_0} = \frac{\sqrt{n}\bar{y}}{\sqrt{\frac{1}{n-1}} \|\boldsymbol{y} - \bar{y}\mathbf{1}_n\|^2}.$$
 (20)

According to the theory above, this test statistic has a null distribution of t_{n-1} .

Example: Two-sample model. Suppose we have $x_1 \in \{0, 1\}$, in which case the linear regression $y = \beta_0 + \beta_1 x_1 + \epsilon$ becomes a two-sample model. We can rewrite this model as

$$y_i \sim \begin{cases} N(\beta_0, \sigma^2) & \text{for } x_i = 0; \\ N(\beta_0 + \beta_1, \sigma^2) & \text{for } x_i = 1. \end{cases}$$
 (21)

It is often of interest to test the null hypothesis $H_0: \beta_1 = 0$, i.e. that the two groups have equal means. Let's define

$$\bar{y}_0 \equiv \frac{1}{n_0} \sum_{i:x_i=0} y_i, \quad \bar{y}_1 \equiv \frac{1}{n_1} \sum_{i:x_i=1} y_i, \quad \text{where} \quad n_0 = |\{i:x_i=0\}| \text{ and } n_1 = |\{i:x_i=1\}|.$$
 (22)

Then, we have seen before that $\hat{\beta}_0 = \bar{y}_0$ and $\hat{\beta}_1 = \bar{y}_1 - \bar{y}_0$. We can compute that

$$s_1^2 \equiv \|\boldsymbol{x}_{*1}^{\perp}\|^2 = \|\boldsymbol{x}_{*1} - \frac{n_1}{n}\boldsymbol{1}\|^2 = n_1 \frac{n_0^2}{n^2} + n_0 \frac{n_1^2}{n^2} = \frac{n_0 n_1}{n} = \frac{1}{\frac{1}{n_0} + \frac{1}{n_1}}$$
(23)

and

$$\widehat{\sigma}^2 = \frac{1}{n-2} \left(\sum_{i:x_i=0} (y_i - \bar{y}_0)^2 + \sum_{i:x_i=1} (y_i - \bar{y}_1)^2 \right). \tag{24}$$

Therefore, we arrive at a t-statistic of

$$t = \frac{\sqrt{\frac{1}{\frac{1}{n_0} + \frac{1}{n_1}}} (\bar{y}_1 - \bar{y}_0)}{\sqrt{\frac{1}{n-2} \left(\sum_{i:x_i=0} (y_i - \bar{y}_0)^2 + \sum_{i:x_i=1} (y_i - \bar{y}_1)^2\right)}}.$$
 (25)

Under the null hypothesis, this statistic has a distribution of t_{n-2} .

t-test for a contrast among coefficients. Given a vector $c \in \mathbb{R}^p$, the quantity $c^T \beta$ is sometimes called a contrast. For example, suppose $c = (1, -1, 0, \dots, 0)$. Then, $c^T \beta = \beta_1 - \beta_2$ is the difference in effects of the first and second predictors. We are sometimes interested in testing whether such a contrast is equal to zero, i.e. $H_0: c^T \beta = 0$. While this hypothesis can involve two or more of the predictors, the parameter $c^T \beta$ is still one-dimensional and therefore we can still apply a t-test. Going back to the distribution $\widehat{\beta} \sim N(\beta, \sigma^2(X^T X)^{-1})$, we find that

$$c^T \widehat{\boldsymbol{\beta}} \sim N(c^T \boldsymbol{\beta}, \sigma^2 c^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} c).$$

Therefore, under the null hypothesis that $c^T \beta = 0$, we can derive that

$$\frac{\boldsymbol{c}^T \widehat{\boldsymbol{\beta}}}{\widehat{\sigma} \sqrt{\boldsymbol{c}^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{c}}} \sim t_{n-p}, \tag{26}$$

giving us another t-test. Note that the t-tests described above can be recovered from this more general formulation by setting $c = e_j$, the indicator vector with jth coordinate equal to 1 and all others equal to zero.

2.2 Testing a multi-dimensional parameter

F-test for a group of coefficients. Now we move on to the case of testing a multi-dimensional parameter: $H_0: \beta_S = \mathbf{0}$ for some $S \subseteq \{0, 1, \dots, p-1\}$. In other words, we would like to test

$$H_0: \mathbf{y} = \mathbf{X}_{*,-S}\boldsymbol{\beta}_{-S} + \boldsymbol{\epsilon} \quad \text{versus} \quad H_1: \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}.$$
 (27)

To test this hypothesis, let us fit least squares coefficients $\hat{\beta}_{-S}$ and $\hat{\beta}$ for the partial model as well as the full model. If the partial model fits well, then the residuals $y - X_{*,-S}\hat{\beta}_{-S}$ from this model will not be much larger than the residuals $y - X\hat{\beta}$ from the full model. To quantify this intuition, let us recall our analysis of variance decomposition from Unit 1:

$$\|\mathbf{y} - \mathbf{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2 = \|\mathbf{X}\widehat{\boldsymbol{\beta}} - \mathbf{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2 + \|\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}\|^2.$$
 (28)

Let's consider the ratio

$$\frac{\|\boldsymbol{y} - \boldsymbol{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2 - \|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2}{\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2} = \frac{\|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2}{\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2},$$
(29)

which is the relative increase in the residual sum of squares when going from the full model to the partial model. Let us rewrite this ratio in terms of projection matrices. Let \boldsymbol{H} be the projection matrix for the full model, and let \boldsymbol{H}_{-S} be the projection matrix for the partial model. Note that $\boldsymbol{H} - \boldsymbol{H}_{-S}$ is the projection matrix onto the |S|-dimensional space $C(\boldsymbol{X}) \cap C(\boldsymbol{X}_{-S})^T$. We have

$$\frac{\|\boldsymbol{X}\widehat{\boldsymbol{\beta}} - \boldsymbol{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2}{\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2} = \frac{\|(\boldsymbol{H} - \boldsymbol{H}_{-S})\boldsymbol{y}\|^2}{\|(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}\|^2}.$$
(30)

Under the null hypothesis, we have

$$\frac{\|(\boldsymbol{H} - \boldsymbol{H}_{-S})\boldsymbol{y}\|^2}{\|(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}\|^2} = \frac{\|(\boldsymbol{H} - \boldsymbol{H}_{-S})\boldsymbol{\epsilon}\|^2}{\|(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{\epsilon}\|^2}.$$
 (31)

Since the projection matrices in the numerator and denominator project onto orthogonal subspaces, we have $(\boldsymbol{H} - \boldsymbol{H}_{-S})\boldsymbol{\epsilon} \perp \!\!\! \perp (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{\epsilon}$, with $\|(\boldsymbol{H} - \boldsymbol{H}_{-S})\boldsymbol{\epsilon}\|^2 \sim \sigma^2 \chi_{|S|}^2$ and $\|(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{\epsilon}\|^2 \sim \sigma^2 \chi_{n-p}^2$.

Renormalizing numerator and denominator to have expectation 1 under the null, we arrive at the F-statistic

$$F \equiv \frac{(\|\boldsymbol{y} - \boldsymbol{X}_{*,-S}\widehat{\boldsymbol{\beta}}_{-S}\|^2 - \|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2)/|S|}{\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2/(n-p)}.$$
 (32)

We have derived that under the null hypothesis,

$$F \sim \frac{\chi_{|S|}^2/|S|}{\chi_{n-p}^2/(n-p)}$$
, with numerator and denominator independent. (33)

This distribution is called the F-distribution with |S| and n-p degrees of freedom, and denoted $F_{|S|,n-p}$. Denoting by $F_{|S|,n-p}(1-\alpha)$ the $1-\alpha$ quantile of this distribution, we arrive at the F-test

$$\phi_F(\boldsymbol{X}, \boldsymbol{y}) \equiv \mathbb{1}(F > F_{|S|, n-p}(1-\alpha)). \tag{34}$$

Example: Testing for any significant coefficients except the intercept. Suppose $x_{*,0} = \mathbf{1}_n$ is an intercept term. Then, consider the null hypothesis $H_0: \beta_1 = \cdots = \beta_{p-1} = 0$. In other words, the null hypothesis is the intercept-only model and the alternative hypothesis is the regression model with an intercept and p-1 additional predictors. In this case, $S = \{1, \ldots, p-1\}$ and $S = \{0\}$. The corresponding F statistic is

$$F \equiv \frac{(\|\boldsymbol{y} - \bar{y}\boldsymbol{1}\|^2 - \|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2)/(p-1)}{\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2/(n-p)},$$
(35)

with null distribution $F_{p-1,n-p}$.

Example: Testing for equality of group means in C**-groups model.** As a further special case, consider the C-groups model from Unit 1. Recall the ANOVA decomposition

$$\sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} (\bar{y}_{c(i)} - \bar{y})^2 + \sum_{i=1}^{n} (y_i - \bar{y}_{c(i)})^2 = SSB + SSW.$$
 (36)

The F-statistic in this case becomes

$$F = \frac{\sum_{i=1}^{n} (\bar{y}_{c(i)} - \bar{y})^2 / (C - 1)}{\sum_{i=1}^{n} (y_i - \bar{y}_{c(i)})^2 / (n - C)} = \frac{SSB/(C - 1)}{SSW/(n - C)},$$
(37)

with null distribution $F_{C-1,n-C}$.

2.3 Power

3 Confidence and prediction intervals

4 R demo