Notes on STAT-331: Applied Linear Models

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Chapter 1. Simple Linear Regression

Section 1. Overview

1.1. Suppose we are given a set of data points $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

- How do we characterize the relationship between x and y?
- How do we predict y given x?
- How does the mean of y change when x increases by a?

We can answer questions like these with **simple linear regression** (SLR):

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i.$$

Intuitively, we are assuming that there exists some underlying linear relationship between the **covariate** x_i and the **outcome** y_i, where the **regression coefficients** β_0 and β_1 are unknown. The **error term** ε_i captures the difference between the actual value of y_i and our prediction $\beta_0 + \beta_1 x_i$.

1.2. The model above is "simple" because there is only one explanatory variable x. Suppose now each sample x_i has three covariates x_{i1}, x_{i2}, and x_{i3}. We generalize SLR to **multiple linear regression** (MLR), where each covariate x_{ij} has a corresponding β_j parameter:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \varepsilon_i,$$

The meaning of y_i and ε_i remain the same; we just have more covariates to work with.

1.3. This course will focus on developing regression models in the following aspects:

- theoretically/mathematically: derive estimators;
- practically: how to fit these models in R;
- how to choose and compare a model, i.e., which covariates to include;
- how to evaluate the appropriateness of the model and assumptions.

Section 2. Simple Linear Regression

1.4. Remark: We make the following assumptions (acronym: LINE):

- **L**inearity: there exists a linear relationship between x and y.
- **I**ndependence: the error terms $\varepsilon_1, \dots, \varepsilon_n$ are independent.
- **N**ormality: the error terms have mean 0.
- **E**qual variance (aka **homoskedasticity**): all error terms share the same variance σ^2.

1.5. Definition: The general form of simple linear regression is given by

$$\boxed{y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \qquad \varepsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2).}$$

- $\beta_0, \beta_1, \sigma^2$: fixed, *unknown* parameters.
- ε_i: *unobserved* random error term.
- y_i, x_i are observed data (we treat x_i as fixed in this course).

Equivalently, we can write

$$\boxed{y_i \overset{\text{indep}}{\sim} N(\beta_0 + \beta_1 x_i, \sigma^2).}$$

Note here y_i's are independent but no longer have the same distribution because they have different means (depending on x_i).

1.6. Example: How to interpret β_0 and β_1? We make the following observations:

1. $\mathbb{E}[y_i \mid x_i] = \beta_0 + \beta_1 x_i$.
2. $\mathbb{E}[y_i \mid x_i = 0] = \beta_0$.
3. $\mathbb{E}[y_i \mid x_i = x^*] = \beta_0 + \beta_1 x^*$.
4. $\mathbb{E}[y_i \mid x_i = x^* + 1] = \beta_0 + \beta_1 (x^* + 1) = \beta_0 + \beta_1 x^* + \beta_1$.
5. $\mathbb{E}[y_i \mid x_i = x^* + 1] - \mathbb{E}[y_i \mid x_i = x^*] = \beta_1$.

Therefore,

- By observation 2, β_0 is the average outcome when $x_0 = 0$.
- By observation 5, β_1 is the expected/average change in y when x moves by 1 unit.

Section 3. SLR: Estimation

1.7. Theorem: *The LS estimators for β_0 and β_1 are given by*

$$\boxed{\begin{aligned}\hat{\beta}_0^{LS} &= \bar{y} - \hat{\beta}_1^{LS}\bar{x} \\ \hat{\beta}_1^{LS} &= \frac{(\sum_i x_i y_i) - n\bar{x}\bar{y}}{(\sum_i x_i^2) - n\bar{x}^2} = \frac{S_{xy}}{S_{xx}}\end{aligned}}$$

Proof. The goal is to choose β_0 and β_1 that minimizes the sum of squared errors given by

$$S(\beta_0, \beta_1) := \sum_{i=1}^{n} \varepsilon_i = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

Differentiate, set the partial derivatives to 0, and solve for β_0 and β_1:

$$\begin{aligned}\frac{\partial S(\delta_0, \delta_1)}{\partial \beta_0} &= \sum_{i=1}^{n} 2(y_i - \beta_0 - \beta_1 x_i)(-1) \\ \frac{\partial S(\delta_0, \delta_1)}{\partial \beta_1} &= \sum_{i=1}^{n} 2(y_i - \beta_0 - \beta_1 x_i)(-x_i)\end{aligned}$$

$$\begin{aligned}\text{(Set) } 0 &= \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) \\ &= \left(\sum_{i=1}^{n} y_i\right) - n\beta_0 - \left(\beta_1 \sum_{i=1}^{n} x_i\right) \\ \implies \beta_0 &= \left(\frac{1}{n}\sum_{i=1}^{n} y_i\right) - \beta_1\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right) = \bar{y} - \beta_1 \bar{x}\end{aligned}$$

$$\begin{aligned}\text{(Set) } 0 &= \sum_{i=1}^{n} (y_i x_i - \beta_0 x_i - \beta_1 x_i^2) \\ &= \left(\sum_{i=1}^{n} y_i x_i\right) - \left(\beta_0 \sum_{i=1}^{n} x_i\right) - \left(\beta_1 \sum_{i=1}^{n} x_i^2\right) \\ &= \left(\sum_{i=1}^{n} y_i x_i\right) - (\bar{y} - \beta_1 \bar{x})n\bar{x} - \left(\beta_1 \sum_{i=1}^{n} x_i^2\right) && \text{plug in previous result} \\ &= \left(\sum_{i=1}^{n} y_i x_i\right) - n\bar{y}\bar{x} + \beta_1 n\bar{x}^2 - \left(\beta_1 \sum_{i=1}^{n} x_i^2\right) \\ &= \left(\sum_{i=1}^{n} y_i x_i\right) - n\bar{y}\bar{x} + \beta_1\left(n\bar{x}^2 - \sum_{i=1}^{n} x_i^2\right) \\ \implies \beta_1 &= \frac{(\sum_{i=1}^{n} y_i x_i) - n\bar{y}\bar{x}}{(\sum_{i=1}^{n} x_i^2) - n\bar{x}^2} = \frac{S_{xy}}{S_{xx}} && \text{See Proposition 1.24}\end{aligned}$$

□

1.8. Theorem: *The ML estimators for β_0 and β_1 coincide with the LS estimators.*

Proof. The **joint likelihood function** of $Y_1, \dots, Y_n$ with $Y_i \overset{\text{indep}}{\sim} N(\beta_0 + \beta_1 x_i, \sigma^2)$ is

$$\begin{aligned} L(\beta_0, \beta_1, \sigma) &= \prod_{i=1}^{n} f(y_i; \beta_0 + \beta_1 x_i, \sigma^2) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \beta_0 - \beta_1 x_i)^2 \right). \end{aligned}$$

The **log-likelihood function** is given by

$$\ell(\beta_0, \beta_1, \sigma^2) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2.$$

Maximizing the log-likelihood is equivalent to solving the following system of equations:

$$\begin{aligned} \frac{\partial \ell}{\partial \beta_0} &= \frac{1}{\sigma^2}\left(\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) \right) = 0 \\ \frac{\partial \ell}{\partial \beta_1} &= \frac{1}{\sigma^2}\left(\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) \right) x_i = 0 \\ \frac{\partial \ell}{\partial \sigma^2} &= -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2}\left(\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) \right)^2 = 0 \end{aligned}$$

Observe solving the first two equations is equivalent to minimizing the sum of squares! In other words, the ML estimators $\hat\beta_0^{\text{ML}}, \hat\beta_1^{\text{ML}}$ coincide with the LS estimators $\hat\beta_0^{\text{LS}}, \hat\beta_1^{\text{LS}}$. Therefore, we will remove the superscripts and simply call them $\hat\beta_0$ and $\hat\beta_1$. □

1.9. Definition: The **fitted values** $\hat y_i$ and the **residuals** e_i are given by

- $\hat y_i = \hat\beta_0 + \hat\beta_1 x_i$.
- $e_i = y_i - \hat y_i = y_i - (\hat\beta_0 + \hat\beta_1 x_i)$.

Note the residuals e_i and the errors $\varepsilon_i = y_i - (\beta_0 + \beta_1 x_i)$ are not the same thing.

1.10. Remark: Solving the third equation, we obtain the ML estimator for σ^2:

$$\hat\sigma^2_{\text{ML}} = \frac{\sum_{i=1}^{n} e_i^2}{n}.$$

This is slightly different from the unbiased estimator for σ^2 (notice the $n-2$ in the denominator):

$$\boxed{\hat\sigma^2 = \frac{\sum_{i=1}^{n} e_i^2}{n-2}.}$$

This difference often doesn't matter when $n \geq 50$.

Section 4. SLR: Inference

1.11. Theorem: *The estimator $\hat\beta_1$ follows the Normal distribution with parameters*

$$\boxed{\hat\beta_1 \sim N\left(\beta_1, \frac{\sigma^2}{S_{xx}}\right).}$$

Proof. Recall $y_i \overset{\text{indep}}{\sim} N(\beta_0 + \beta_1 x_i, \sigma^2)$. Let us rewrite $\hat\beta_1$ as

$$\begin{aligned}
\hat\beta_1 = \frac{S_{xy}}{S_{xx}} &= \frac{\sum_i (y_i - \bar y)(x_i - \bar x)}{\sum_i (x_i - \bar x)^2} \\
&= \frac{\sum_i y_i (x_i - \bar x)}{\sum_i (x_i - \bar x)^2} =: \sum_{i=1}^n w_i y_i, \qquad\qquad w_i := \frac{(x_i - \bar x)}{\sum_i (x_i - \bar x)}.
\end{aligned}$$

Since we assumed that x_i's are fixed, the variables w_i's are fixed wrt the y_i's. Thus, $\hat\beta_1$ is a linear combination independent Normal random variables $y_1, \ldots, y_n$. Moreover, all y_i's share the same variance (homoskedasticity). By the Fact above, β_i follows the normal distribution with parameters

$$\hat\beta_1 \sim N\left(\sum_{i=1}^n w_i(\beta_0 + \beta_1 x_i), \sigma^2 \sum_{i=1}^n w_i^2\right).$$

It remains to simplify the parameters.

$$\begin{aligned}
\mathbb{E}[\hat\beta_1] &= \sum_{i=1}^n w_i \left(\beta_0 + \beta_1 x_i\right) \\
&= \sum_{i=1}^n \frac{(x_i - \bar x)}{\sum (x_i - \bar x)^2} \left(\beta_0 + \beta_1 x_i\right) \\
&= \beta_0 \frac{\sum_{i=1}^n (x_i - \bar x)}{\sum (x_i - \bar x)^2} + \beta_1 \frac{\sum_{i=1}^n x_i (x_i - \bar x)}{\sum (x_i - \bar x)^2} \\
&= 0 + \beta_1 \frac{\sum_{i=1}^n (x_i - \bar x)(x_i - \bar x)}{\sum (x_i - \bar x)^2} = \beta_1 \qquad\qquad \sum_{i=1}^n (x_i - \bar x) = 0
\end{aligned}$$

$$\begin{aligned}
\mathrm{Var}[\hat\beta_1] &= \sigma^2 \sum_{i=1}^n w_i^2 \\
&= \sigma^2 \sum_{i=1}^n \left[\frac{(x_i - \bar x)}{\sum_{i=1}^n (x_j - \bar x)^2}\right]^2 \\
&= \sigma^2 \sum_{i=1}^n \frac{(x_i - \bar x)^2}{\left[\sum_{j=1}^n (x_j - \bar x)^2\right]^2} \\
&= \sigma^2 \frac{\sum_{i=1}^n (x_i - \bar x)^2}{\left[\sum_{j=1}^n (x_j - \bar x)^2\right]^2} = \sigma^2 \frac{1}{\sum_{i=1}^n (x_i - \bar x)^2} = \frac{\sigma^2}{S_{xx}}
\end{aligned}$$

□

1.12. Theorem: *The estimator $\hat{\beta}_0$ follows the Normal distribution with parameters*

$$\boxed{\hat{\beta}_0 \sim N\left(\beta_0, \sigma^2\left[\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right]\right).}$$

Proof.

$$\begin{aligned}
\mathbb{E}\left[\hat{\beta}_0\right] &= \mathbb{E}\left[\bar{y} - \hat{\beta}_1\bar{x}\right] = \mathbb{E}[\bar{y}] - \mathbb{E}[\hat{\beta}_1\bar{x}] \\
&= \mathbb{E}\left[\frac{1}{n}\sum_i^n y_i\right] - \bar{x}\mathbb{E}\left[\hat{\beta}_1\right] \\
&= \frac{1}{n}\left(\sum_{i=1}^n \mathbb{E}[y_i]\right) - \bar{x}\beta_1 && \mathbb{E}[\hat{\beta}_1] = \beta_1 \\
&= \frac{1}{n}\left(\sum_{i=1}^n (\beta_0 + \beta_1 x_i)\right) - \bar{x}\beta_1 && \mathbb{E}[y_1] = \beta_0 + \beta_1 x_i \\
&= \beta_0 + \beta_1\bar{x} - \bar{x}\beta_1 = \beta_0
\end{aligned}$$

$$\begin{aligned}
\text{Var}\hat{\beta}_0 &= \text{Var}\left(\bar{y} - \hat{\beta}_1\bar{x}\right) \\
&= \text{Var}(\bar{y}) - 2\text{Cov}\left(\bar{y}, \hat{\beta}_1\bar{x}\right) + \text{Var}\left(\hat{\beta}_1\bar{x}\right) \\
&= \frac{\sigma^2}{n} - 2\bar{x}\text{Cov}\left(\bar{y}, \hat{\beta}_1\right) + \bar{x}^2\text{Var}\hat{\beta}_1 && \text{See } (1.25) \\
&= \frac{\sigma^2}{n} - 2\bar{x}\text{Cov}\left(\bar{y}, \hat{\beta}_1\right) + \bar{x}^2\frac{\sigma^2}{S_{xx}} \\
&= \sigma^2\left[\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right] - 2\bar{x}\text{Cov}\left(\bar{y}, \hat{\beta}_1\right).
\end{aligned}$$

It remains to show that $\text{Cov}(\bar{y}, \hat{\beta}_1) = 0$.

$$\begin{aligned}
\text{Cov}\left(\bar{y}, \hat{\beta}_1\right) &= \text{Cov}\left(\frac{1}{n}\sum_{i=1}^n y_i, \frac{\sum_i (x_i - \bar{x})\, y_i}{\sum_i (x_i - \bar{x})^2}\right) \\
&= \frac{1}{n\sum_i (x_i - \bar{x})^2}\text{Cov}\left(\sum_i Y_i, \sum_i (x_i - \bar{x})\, Y_i\right) \\
&= \frac{1}{n\sum_i (x_i - \bar{x})^2}\sum_{i,j}\text{Cov}\left(y_i, (x_i - \bar{x})\, y_j\right) && \text{Cov}\left(y_i, (x_i - \bar{x})\, y_j\right) \propto \delta_{i,j} \\
&= \frac{1}{n\sum_i (x_i - \bar{x})^2}\sum_i (x_i - \bar{x})\,\text{Var}(y_i) && \text{Cov}(y_i, y_i) = \text{Var}(y_i) \\
&= \frac{\sigma^2}{n\sum_i (x_i - \bar{x})^2}\sum_i (x_i - \bar{x}) && \text{Var}(y_i) = \sigma^2 \\
&= 0 && \sum_i (x_i - \bar{x}) = 0
\end{aligned}$$

□

Section 5. SLR: Confidence Interval

1.13. Let us derive a 95% confidence interval for β_1. Recall that

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{S_{xx}}\right) \implies Z := \frac{\hat{\beta}_1 - \beta_1}{\sigma/\sqrt{S_{xx}}} \sim N(0,1). \tag{1.1}$$

Suppose σ is known. Then

$$\begin{aligned} 0.95 &= P(-1.96 \leq Z \leq 1.96) \\ &= P\left(-1.96 \leq \frac{\hat{\beta}_1 - \beta_1}{\sigma/\sqrt{S_{xx}}} \leq 1.96\right) \\ &= P\left(-1.96\frac{\sigma}{\sqrt{S_{xx}}} \leq \hat{\beta}_1 - \beta_1 \leq 1.96\frac{\sigma}{\sqrt{S_{xx}}}\right) \\ &= P\left(-1.96\frac{\sigma}{\sqrt{S_{xx}}} \leq \beta_1 - \hat{\beta}_1 \leq 1.96\frac{\sigma}{\sqrt{S_{xx}}}\right) \\ &= P\left(\hat{\beta}_1 - 1.96\frac{\sigma}{\sqrt{S_{xx}}} \leq \beta_1 \leq \hat{\beta}_1 + 1.96\frac{\sigma}{\sqrt{S_{xx}}}\right) \end{aligned}$$

Thus, a 95% CI for β_1 is

$$\hat{\beta}_1 \pm 1.96\frac{\sigma}{\sqrt{S_{xx}}}.$$

In practice, σ^2 is often unknown. We can estimate it using the unbiased estimator $\hat{\sigma}^2$.

1.14. Definition: The **standard error** $\mathrm{SE}(\hat{\beta}_1)$ is an estimator of $\hat{\beta}_1$'s standard deviation:

$$\boxed{\mathrm{SE}(\hat{\beta}_1) := \sqrt{\frac{\hat{\sigma}^2}{S_{xx}}} = \frac{\hat{\sigma}}{\sqrt{S_{xx}}}.}$$

1.15. Theorem: *The confidence interval of $\hat{\beta}_1$ is given by*

$$\boxed{\hat{\beta}_1 \pm t_{1-\alpha/2,n-2}\mathrm{SE}(\hat{\beta}_1).}$$

Proof. Replacing σ^2 by $\hat{\sigma}^2$ in (1.1) gives the t-distributed pivotal quantity

$$\frac{\hat{\beta}_1 - \beta_1}{\hat{\sigma}/\sqrt{S_{xx}}} = \frac{\hat{\beta}_1 - \beta_1}{\mathrm{SE}(\hat{\beta}_1)} \sim t_{(n-2)}.$$

A $100(1-\alpha)\%$ confidence interval is given by

$$1-\alpha = \Pr\left(-q \leq \frac{\hat{\beta}_1 - \beta_1}{\mathrm{SE}(\hat{\beta}_1)} \leq q\right) = \Pr\left(\hat{\beta}_1 - q\frac{\hat{\sigma}}{\mathrm{SE}(\hat{\beta}_1)} \leq \beta_1 \leq \hat{\beta}_1 + q\frac{\hat{\sigma}}{\mathrm{SE}(\hat{\beta}_1)}\right)$$

Thus, a 95% CI for β_1 is

$$\hat{\beta}_1 \pm t_{1-\alpha/2,n-2}\frac{\hat{\sigma}}{\sqrt{S_{xx}}}$$

where $t_{1-\alpha/2,n-2}$ is can be found with `qt(p = alpha/2, df = n-2)` in R. □

Section 6. SLR: Hypotheses Testing

1.16. Suppose we want to test a null hypothesis $H_0 : \beta_1 = \theta_0$ against some alternative hypothesis $H_1 : \beta_1 \neq \theta_0$. For SLR, we often set

- $H_0 : \beta_1 = 0$: no linear relationship;
- $H_1 : \beta_1 \neq 0$: two-sided alternative.

The goal is to characterize how much evidence we have against H_0, or how "extreme" our data are relative to H_0. We can test the null hypothesis with the t-statistic

$$T := \frac{\hat{\beta}_1 - \theta_0}{\hat{\sigma}/\sqrt{S_{xx}}} \sim t_{(n-2)}.$$

Assuming H_0 is true, what's the probability to have some as extreme or more than what we observe?

$$\Pr(|T| \geq |t_{\text{obs}}|) = 2\Pr(T \geq |t_{\text{obs}}|) = 2[1 - \Pr(T \leq -|t_{\text{obs}}|)].$$

We typically reject the null hypothesis at the 5% level, i.e., reject H_0 if $p < 0.05$. Would we accept H_0 if $p > 0.05$? **No, we simply would not have enough evidence to reject.**

1.17. Remark: Does this mean $\Pr(\beta_1 = 0) = p$? No. Instead, it means under the null hypothesis, i.e., assuming $\beta_1 = 0$, the probability of a test statistic as extreme as the one observed is equal to p. That's why a small p-value is evidence against the null, since it would be particularly "rare" under the null.

1.18. Remark: Note that a $100(1-\alpha)\%$ CI (e.g., 0.95) corresponds with a hypothesis test with a $100\alpha\%$ significance level (e.g., 0.05), i.e., we will derive a similar conclusion. In particular, if we reject H_0 at the 0.05-level (i.e., when the p-value is less than 0.05), then the 95% CI will not contain the value of 0.

Section 7. SLR: Estimation of Mean Response

1.19. Theorem: *Given new x_0, the estimated mean response is given by*

$$\hat{\mu}_0 = \beta_0 + \beta_1 x_0 \sim N\left(\mu_0, \sigma^2\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^n (x_i-\bar{x})^2}\right)\right).$$

Proof. The mean response for an arbitrary x_0 is given by

$$\hat{\mu}_0 = \mathbb{E}[y \mid x_0] = \hat{\beta}_0 + \hat{\beta}_1 x_0 = (\bar{y} - \hat{\beta}_1 \bar{x}) + \hat{\beta}_1 x_0 = \bar{y} + \hat{\beta}_1 (x_0 - \bar{x}).$$

The estimate of mean response is unbiased:

$$\mathbb{E}[\hat{\mu}_0] = \mathbb{E}[\hat{\beta}_0 + \hat{\beta}_1 x_0] = \mathbb{E}[\hat{\beta}_0] + \mathbb{E}[\hat{\beta}_1] x_0 = \beta_0 + \beta_1 x_0 =: \mu_0.$$

The variance is given by

$$\begin{aligned}
\mathrm{Var}\left[\hat{\mu}_0\right] &= \mathrm{Var}\left[\hat{\beta}_0 + \hat{\beta}_1 x_0\right] \\
&= \mathrm{Var}\left[\left(\bar{y} - \hat{\beta}_1 \bar{x}\right) + \hat{\beta}_1 x_0\right] \\
&= \mathrm{Var}\left[\bar{y} + \hat{\beta}_1 \left(x_0 - \bar{x}\right)\right] \\
&= \mathrm{Var}\left[\left(\sum_{i=1}^n \frac{1}{n} y_i\right) + \left(\sum_{i=1}^n \frac{(x_i-\bar{x})}{S_{xx}} y_i\right)\left(x_0 - \bar{x}\right)\right] \\
&= \mathrm{Var}\left[\sum_{i=1}^n \left(\frac{1}{n} + \frac{\left(x_i-\bar{x}\right)\left(x_0-\bar{x}\right)}{S_{xx}}\right) y_i\right] \qquad \star \\
&= \sum_{i=1}^n \left(\frac{1}{n} + \frac{\left(x_i-\bar{x}\right)\left(x_0-\bar{x}\right)}{S_{xx}}\right)^2 \sigma^2 \\
&= \sigma^2 \sum_{i=1}^n \left(\frac{1}{n^2} + \frac{\left(x_i-\bar{x}\right)^2\left(x_0-\bar{x}\right)^2}{S_{xx}^2} + 2\frac{1}{n}\frac{\left(x_i-\bar{x}\right)\left(x_0-\bar{x}\right)}{S_{xx}}\right) \\
&= \sigma^2 \left(\sum_{i=1}^n \frac{1}{n^2} + \sum_{i=1}^n \frac{\left(x_i-\bar{x}\right)^2\left(x_0-\bar{x}\right)^2}{S_{xx}^2} + 2\sum_{i=1}^n \frac{1}{n}\frac{\left(x_i-\bar{x}\right)\left(x_0-\bar{x}\right)}{S_{xx}}\right) \\
&= \sigma^2 \left(\frac{1}{n} + \frac{\left(x_0-\bar{x}\right)^2}{S_{xx}^2} S_{xx} + 2\frac{1}{n}\frac{\left(x_0-\bar{x}\right)}{S_{xx}} \sum_{i=1}^n \left(x_i - \bar{x}\right)\right) \\
&= \sigma^2 \left(\frac{1}{n} + \frac{\left(x_0-\bar{x}\right)^2}{\sum_{i=1}^n \left(x_i-\bar{x}\right)^2}\right)
\end{aligned}$$

Note in the 5th line of the derivation of variance (labeled $\star$), we see that $\hat{\mu}_0$ is a linear combination of Normal random variables y_i, so μ_0 is also Normal:

$$\hat{\mu}_0 \sim N\left(\mu_0, \sigma^2\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^n (x_i-\bar{x})^2}\right)\right).$$

□

1.20. Note: From above, we know that

$$\frac{\hat{\mu}_0 - \mu_0}{\sigma\sqrt{\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)}} \sim N(0,1) \quad \text{and} \quad \frac{\hat{\mu}_0 - \mu_0}{\hat{\sigma}\sqrt{\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)}} \sim t_{n-2}.$$

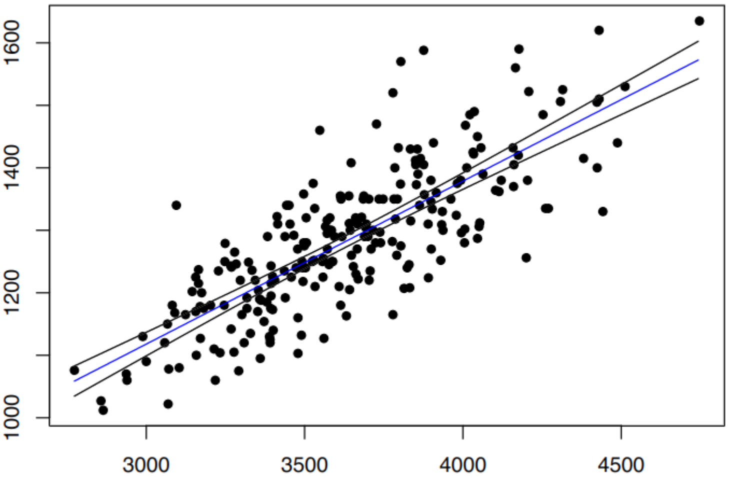
Thus, a 95% CI is given by

$$0.95 = P\left(-t_{n-2,1-\frac{\alpha}{2}} \leq \frac{\hat{\mu}_0 - \mu_0}{\hat{\sigma}\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)^{1/2}} \leq t_{n-2,1-\frac{\alpha}{2}}\right)$$

In general, a $100(1-\alpha)\%$ CI is given by

$$\boxed{\hat{\mu}_0 \pm t_{n-2,1-\frac{\alpha}{2}}\hat{\sigma}\sqrt{\left(\frac{1}{n} + \frac{(x_0-\bar{x})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)}.}$$

Note that the CIs get bigger as $x \to \infty$ and $x \to -\infty$ as we have fewer data points there.



Note that many points fall outside of the CI. What if we don't just care about the mean, but also the predictions? That is, even if we got the mean absolutely perfect, the new points wouldn't fall directly on the line!

Section 8. SLR: Prediction of a Single Response

1.21. Note: Suppose we want to predict the response for a new covariate value:

$$y_{\text{new}} = \beta_0 + \beta_1 x_{\text{new}} + \varepsilon_{\text{new}}.$$

Define the predicted value $\hat{y}_{\text{new}} = \hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}$ and prediction error $\hat{y}_{\text{new}} - y_{\text{new}}$. Let's quantify the prediction error.

$$\begin{aligned} E\left[\hat{y}_{\text{new}} - y_{\text{new}}\right] &= E\left[\left(\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}\right) - \left(\beta_0 + \beta_1 x_{\text{new}} + \varepsilon_{\text{new}}\right)\right] \\ &= \beta_0 + \beta_1 x_{\text{new}} - \left(\beta_0 + \beta_1 x_{\text{new}}\right) = 0 \end{aligned}$$

Note that $\hat{y}_{\text{new}}$ and y_{new} are independent, because the former is a linear combination of the known y_i's while the latter has nothing to do with those. Moreover, $\hat{y}_{\text{new}}$ is Normal as y_i's are Normal.

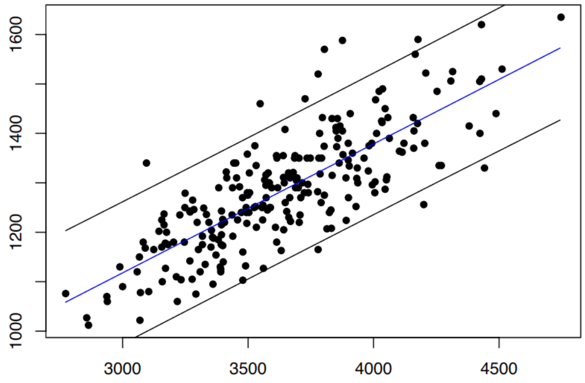
$$\begin{aligned} \text{Var}\left[\hat{y}_{\text{new}} - y_{\text{new}}\right] &= \text{Var}\left[\left(\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}\right) - y_{\text{new}}\right] \\ &= \text{Var}\left[\left(\hat{\beta}_0 + \hat{\beta}_1 x_{\text{new}}\right)\right] + \text{Var}\left[y_{\text{new}}\right] \\ &= \left[\sigma^2\left(\frac{1}{n} + \frac{\left(x_{\text{new}} - \bar{x}\right)^2}{\sum_{i=1}^n \left(x_i - \bar{x}\right)^2}\right)\right] + \left[\sigma^2\right] \\ &= \sigma^2\left(1 + \frac{1}{n} + \frac{\left(x_{\text{new}} - \bar{x}\right)^2}{\sum_{i=1}^n \left(x_i - \bar{x}\right)^2}\right) \end{aligned}$$

Using the same approach as above, we have

$$\frac{\hat{y}_{\text{new}} - y_{\text{new}}}{\sigma\sqrt{\left(1 + \frac{1}{n} + \frac{\left(x_{\text{new}} - \bar{x}\right)^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right)}} \sim N(0,1) \quad \text{and} \quad \frac{\hat{y}_{\text{new}} - y_{\text{new}}}{\hat{\sigma}\sqrt{\left(1 + \frac{1}{n} + \frac{\left(x_{\text{new}} - \bar{x}\right)^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right)}} \sim t_{n-2}.$$

Thus, a $100(1-\alpha)\%$ **prediction interval** is given by

$$\boxed{\hat{y}_{\text{new}} \pm t_{n-2,\left(1-\frac{\alpha}{2}\right)}\hat{\sigma}\sqrt{\left(1 + \frac{1}{n} + \frac{\left(x_{\text{new}} - \bar{x}\right)^2}{\sum_{i=1}^n \left(x_i - \bar{x}\right)^2}\right)}.}$$



Note the margin of error of PI is much wider compared to the previous CI.

Section 9. Appendix

1.22. Definition: Let $\bar{x}, \bar{y}$ denote the mean of x's and y's. Define

$$\boxed{\begin{aligned} S_{xx} &= \sum_{i=1}^{n} (x_i - \bar{x})^2 \\ S_{xy} &= \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) \\ S_{yy} &= \sum_{i=1}^{n} (y_i - \bar{y})^2 \end{aligned}}$$

1.23. Lemma: *Let $\bar{x}$ be the mean of $\{x_1, \ldots, x_n\}$. Then*

$$\boxed{\sum_{i=1}^{n} (x_i - \bar{x}) = 0.}$$

Proof. Observe that

$$\begin{aligned} \sum_{i=1}^{n} (x_i - \bar{x}) &= \left[\sum_{i=1}^{n} x_i\right] - n\bar{x} \\ &= \left[\sum_{i=1}^{n} x_i\right] - n\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right) = \left[\sum_{i=1}^{n} x_i\right] - \left[\sum_{i=1}^{n} x_i\right] = 0. \end{aligned}$$

□

1.24. Proposition: *We have the following equalities for S_{xx} and S_{xy}:*

$$\boxed{\begin{aligned} S_{xx} &= \left(\sum_{i=1}^{n} x_i^2\right) - n\bar{x}^2 \\ S_{xy} &= \left(\sum_{i=1}^{n} x_i y_i\right) - n\bar{x}\bar{y}. \end{aligned}}$$

Proof. Observe that

$$\begin{aligned} S_{xx} &= \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x}) \\ &= \left[\sum_{i=1}^{n} x_i(x_i - \bar{x})\right] - \left[\bar{x}\sum_{i=1}^{n} (x_i - \bar{x})\right] && \bar{x} \text{ does not depend on } i \\ &= \sum_{i=1}^{n} x_i(x_i - \bar{x}) && \sum_{i=1}^{n} (x_i - \bar{x}) = 0 \end{aligned}$$

$$
\begin{aligned}
&= \left[\sum_{i=1}^{n} x_i^2\right] - \left[\bar{x}\sum_{i=1}^{n} x_i\right] && \bar{x} \text{ does not depend on } i \\
&= \left[\sum_{i=1}^{n} x_i^2\right] - \bar{x}(n\bar{x}) && \bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \implies \sum_{i=1}^{n} x_i = n\bar{x} \\
&= \left[\sum_{i=1}^{n} x_i^2\right] - n\bar{x}^2
\end{aligned}
$$

The second property can be derived using a similar approach (Exercise). □

1.25. Lemma:

$$\operatorname{Var}(\bar{X}) = \operatorname{Var}\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{1}{n^2}\sum_{i=1}^{n}\operatorname{Var}(X_i) = \frac{1}{n^2}n\sigma^2 = \frac{\sigma^2}{n}$$

Chapter 2. Multiple Linear Regression

Chapter Highlight

Let $\mathbf{y} = (y_1, \ldots, y_n)$ be a random vector. Then

$$\boxed{\begin{aligned} \mathbb{E}[\mathbf{y}] &= [\mathbb{E}[y_i]]_{1\leq i\leq n} \in \mathbb{R}^{n\times 1}, \\ \mathrm{Var}[\mathbf{y}] &= [\mathrm{Cov}(y_i, y_j)]_{1\leq i,j\leq n} \in \mathbb{R}^{n\times n}. \end{aligned}}$$

In particular, V is *symmetric* and *positive semidefinite*.

Properties of $\mathbb{E}$, Var, and Cov:

$$\boxed{\begin{aligned} \mathbb{E}[\mathbf{a}^T\mathbf{y} + c] &= a^T\boldsymbol{\mu} + c \in \mathbb{R} \\ \mathrm{Cov}(\mathbf{a}^T\mathbf{y} + c, \mathbf{b}^T\mathbf{y} + d) &= \mathbf{a}^T\mathbf{V}\mathbf{b} \in \mathbb{R} \\ \mathbb{E}[\mathbf{A}\mathbf{y} + \mathbf{b}] &= \mathbf{A}\mathbb{E}[\mathbf{y}] + \mathbf{b} = \mathbf{A}\boldsymbol{\mu} \in \mathbb{R}^k \\ \mathrm{Var}(\mathbf{A}\mathbf{y} + \mathbf{b}) &= \mathbf{A}\mathrm{Var}(\mathbf{y})\mathbf{A}^T = \mathbf{A}\mathbf{V}\mathbf{A}^T \in \mathbb{R}^{k\times k}. \end{aligned}}$$

Section 1. Review: Linear Algebra and Calculus

2.1. Remark: It's often a lot easier to understand formulas intuitively in higher-dimensional spaces once you know their sizes/dimensions (sanity check!). I will try to label the dimensions of vectors and spaces as much as possible. **Warning**: There will be abuse of notations for random variables, e.g., I will label a random vector $\mathbf{x}$ with three elements as $\mathbf{x} \in \mathbb{R}^3$.

2.2. Note: We briefly review some facts about matrices. Let $\mathbf{A}, \mathbf{B}, \mathbf{C}$ be matrices.

- $[\mathbf{C}^T]_{ij} = [\mathbf{C}]_{ij}$.
- $\mathbf{C}$ is **symmetric** if $\mathbf{C}^T = \mathbf{C}$.
- $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$.
- If a square matrix $\mathbf{B}$ is non-singular, then $\mathbf{BB}^{-1} = \mathbf{B}^{-1}\mathbf{B} = \mathbf{I}$.
- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$ is both are non-singular square matrices.
- $(\mathbf{A}^T)^{-1} = (\mathbf{A}^{-1})^T$.
- $\mathrm{tr}(\mathbf{A}) = \sum_j^n a_{jj}$ for square matrix $\mathbf{A}$.
- $\mathrm{tr}(c\mathbf{A} + \mathbf{B}) = c \cdot \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B})$.
- $\mathrm{tr}(\mathbf{A}^T) = \mathrm{tr}(\mathbf{A})$.
- $\mathrm{tr}(\mathbf{AB}) = \mathrm{tr}(\mathbf{BA})$.

2.3. Note: We briefly review some matrix calculus.

- Let $\mathbf{y} = (y_1, \dots, y_k) \in \mathbb{R}^k$ and $f : \mathbb{R}^k \to \mathbb{R}$ be a function of $\mathbf{y}$. Then
$$\frac{\partial f}{\partial \mathbf{y}} = \begin{bmatrix} \dfrac{\partial f}{\partial y_1} \\ \vdots \\ \dfrac{\partial f}{\partial y_k} \end{bmatrix} \in \mathbb{R}^{k\times 1}$$
- If $z = \mathbf{a}^T\mathbf{y} \in \mathbb{R}$ where $\mathbf{a} = (a_1, \dots, a_k) \in \mathbb{R}^k$ is a column vector, then
$$\frac{\partial z}{\partial \mathbf{y}} = \mathbf{a} \in \mathbb{R}^{k\times 1}.$$
- If $z = \mathbf{y}^T A\mathbf{y} \in \mathbb{R}$ where $A \in \mathbb{R}^{k\times k}$, then
$$\frac{\partial z}{\partial \mathbf{y}} = (A + A^T)\mathbf{y} \in \mathbb{R}^{k\times 1}.$$
  In particular, if A is symmetric, then
$$\frac{\partial z}{\partial \mathbf{y}} = 2A\mathbf{y} \in \mathbb{R}^{k\times 1}.$$

Section 2. Random Vectors

2.4. Definition: A **random vector** is a vector of random variables.
Let $\mathbf{y} = (y_1, \ldots, y_n)$ be a random vector. The **mean** of $\mathbf{y}$ is

$$\boxed{\mathbb{E}[\mathbf{y}] = \begin{bmatrix} \mathbb{E}[y_1] \\ \vdots \\ \mathbb{E}[y_n] \end{bmatrix} \in \mathbb{R}^{n\times 1}.}$$

The **variance** of $\mathbf{y}$ is given by the **covariance matrix**:

$$\begin{aligned} \mathrm{Var}(\mathbf{y}) = \mathbf{V} &= \mathbb{E}[(\mathbf{y}-\boldsymbol{\mu})(\mathbf{y}-\boldsymbol{\mu})^T] \\ &= \begin{bmatrix} \mathrm{Var}(y_1) & \mathrm{Cov}(y_1,y_2) & \cdots & \mathrm{Cov}(y_1,y_n) \\ \mathrm{Cov}(y_2,y_1) & \mathrm{Var}(y_2) & \cdots & \mathrm{Cov}(y_1,y_n) \\ \vdots & \vdots & & \vdots \\ \mathrm{Cov}(y_n,y_1) & \mathrm{Cov}(y_n,y_2) & \cdots & \mathrm{Var}(y_n) \end{bmatrix} \in \mathbb{R}^{n\times n} \end{aligned}$$

In particular,

$$\boxed{\mathbf{V}_{ij} = \mathrm{Cov}(y_i, y_j).}$$

2.5. Proposition: *Let $V = \mathrm{Var}(\mathbf{y})$ be the covariance matrix of $\mathbf{y}$.*

- $\mathbf{V}$ *is* ***symmetric****, i.e.,* $\mathbf{V}_{ij} = \mathbf{V}_{ji}$.
- $\mathbf{V}$ *is* ***positive semidefinite****, i.e.,* $\forall \mathbf{a} \in \mathbb{R}^n$, $\mathbf{a}^T\mathbf{V}\mathbf{a} \geq 0$.

Proof. The first claim follows from the fact that the Cov operator is symmetric. For the second claim, observe that

$$\mathbf{a}^T\mathbf{V}\mathbf{a} = \mathbf{a}^T\mathbb{E}[(\mathbf{y}-\boldsymbol{\mu})(\mathbf{y}-\boldsymbol{\mu})^T]\mathbf{a} = \mathbb{E}[\mathbf{a}^T(\mathbf{y}-\boldsymbol{\mu})(\mathbf{y}-\boldsymbol{\mu})^T\mathbf{a}] \overset{\star}{=} \mathbb{E}[((\mathbf{y}-\boldsymbol{\mu})^T\mathbf{a})^2] \geq 0$$

where $\star$ follows from the fact that $\mathbf{a}^T(\mathbf{y}-\boldsymbol{\mu})$ and $(\mathbf{y}-\boldsymbol{\mu})^T\mathbf{a}$ are scalars. □

2.6. Note: Recall the following facts. Let $a_i, b_i, c, d \in \mathbb{R}$ be constants, y_i be random variables, and $z = \sum_{i=1}^n a_i y_i + c$, $u = \sum_{i=1}^n b_i y_i + d$ be linear combinations of y_i's; $z, u \in \mathbb{R}$. Then

$$\boxed{\begin{aligned} \mathbb{E}[z] &= \sum_{i=1}^n a_i \mathbb{E}[y_i] + c \in \mathbb{R} \\ \mathrm{Cov}(z,u) &= \sum_{i=1}^n \sum_{j=1}^n a_i b_j \mathrm{Cov}(y_i, y_j) \in \mathbb{R}. \end{aligned}}$$

Equivalently in matrix notation, $z = \mathbf{a}^T\mathbf{y} + c \in \mathbb{R}$, $u = \mathbf{b}^T\mathbf{y} + d \in \mathbb{R}$, then

$$\boxed{\begin{aligned} \mathbb{E}[\mathbf{a}^T\mathbf{y} + c] &= a^T\boldsymbol{\mu} + c \in \mathbb{R} \\ \mathrm{Cov}(\mathbf{a}^T\mathbf{y} + c, \mathbf{b}^T\mathbf{y} + d) &= \mathbf{a}^T\mathbf{V}\mathbf{b} \in \mathbb{R} \end{aligned}}$$

where $\boldsymbol{\mu} = \mathbb{E}[\mathbf{y}]$ and $\mathbf{V} = \mathrm{Var}(\mathbf{y})$. We now consider their multivariate counterparts.

2.7. Note: Consider a random vector $\mathbf{z} = (z_1, \dots, z_k)^T$ of k linear combinations of random $\mathbf{y}$:

$$\begin{aligned} z_1 &= a_{11}y_1 + a_{12}y_2 + \cdots + a_{1n}y_n \\ z_2 &= a_{21}y_1 + a_{22}y_2 + \cdots + a_{2n}y_n \\ &\vdots \\ z_k &= a_{k1}y_1 + a_{k2}y_2 + \cdots + a_{kn}y_n \end{aligned}$$

We can equivalently write $\mathbf{z} = \mathbf{A}\mathbf{y} \in \mathbb{R}^k$ for $\mathbf{A} \in \mathbb{R}^{k \times n}$, $[\mathbf{A}]_{ij} = a_{ij}$. Then

$$\begin{aligned} \mathbb{E}[\mathbf{A}\mathbf{y}] &= \mathbf{A}\mathbb{E}[\mathbf{y}] = \mathbf{A}\boldsymbol{\mu} \in \mathbb{R}^k \\ \mathrm{Var}(\mathbf{A}\mathbf{y}) &= \mathbb{E}[(\mathbf{A}\mathbf{y} - \mathbb{E}[\mathbf{A}\mathbf{y}])(\mathbf{A}\mathbf{y} - \mathbb{E}[\mathbf{A}\mathbf{y}])^T] \\ &= \mathbb{E}[\mathbf{A}(\mathbf{y} - \mathbb{E}[\mathbf{y}])(\mathbf{A}(\mathbf{y} - \mathbb{E}[\mathbf{y}]))^T] \\ &= \mathbb{E}[\mathbf{A}(\mathbf{y} - \mathbb{E}[\mathbf{y}])(\mathbf{y} - \mathbb{E}[\mathbf{y}])^T A^T] \\ &= \mathbf{A}\mathbb{E}[(\mathbf{y} - \mathbb{E}[\mathbf{y}])(\mathbf{y} - \mathbb{E}[\mathbf{y}])^T] A^T \\ &= \mathbf{A}\mathrm{Var}(\mathbf{y})\mathbf{A}^T \\ &= \mathbf{A}\mathbf{V}\mathbf{A}^T \in \mathbb{R}^{k \times k} \end{aligned}$$

where $\boldsymbol{\mu} = \mathbb{E}[\mathbf{y}]$ and $\mathbf{V} = \mathrm{Var}(\mathbf{y})$. In other words, you can pull out a matrix of constants from the expectation and the variance operator much like what you do with vectors. We summarize this result into the following proposition (with an extra bias term $\mathbf{b}$).

2.8. Theorem: *Let $y \in \mathbb{R}^n$ and $\mathbf{A} \in \mathbb{R}^{k \times n}$. Then*

$$\boxed{\begin{aligned} \mathbb{E}[\mathbf{A}\mathbf{y} + \mathbf{b}] &= \mathbf{A}\mathbb{E}[\mathbf{y}] + \mathbf{b} = \mathbf{A}\boldsymbol{\mu} \in \mathbb{R}^k \\ \mathrm{Var}(\mathbf{A}\mathbf{y} + \mathbf{b}) &= \mathbf{A}\mathrm{Var}(\mathbf{y})\mathbf{A}^T = \mathbf{A}\mathbf{V}\mathbf{A}^T \in \mathbb{R}^{k \times k}. \end{aligned}}$$

Section 3. Multivariate Normal Distribution

2.9. Definition: A vector $\mathbf{y}$ has a **multivariate normal distribution** $\mathrm{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ if its density function has the form

$$\boxed{f(\mathbf{y}) = \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\left\{ -\frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right\}}$$

where $\mathbb{E}[\mathbf{y}] = \boldsymbol{\mu}$ and $\mathrm{Var}(\mathbf{y}) = \boldsymbol{\Sigma}$.

2.10. Example: Let $\mathbf{z} = (z_1, \ldots, z_n) \in \mathbb{R}^n$ be a random vector of iid standard normal random variables, i.e., $z_i \overset{\text{iid}}{\sim} N(0, 1)$ for all i's. Then for any $\mathbf{A} \in \mathbb{R}^{k \times n}$,

$$\mathbf{y} = \mathbf{A}\mathbf{z} + \boldsymbol{\mu} \in \mathbb{R}^k \sim \mathrm{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma}),$$

where $\mathbb{E}[\mathbf{y}] = \boldsymbol{\mu}$ and $\mathrm{Var}(\mathbf{y}) = \boldsymbol{\Sigma} = \mathbf{A}\mathbf{A}^T$.

2.11. Proposition: *Some nice properties of MVN:*

- *Linearity: If $\mathbf{u} = \mathbf{C}\mathbf{y} + \mathbf{d}$, then*

$$\mathbf{u} \sim MVN(\mathbf{C}\boldsymbol{\mu} + \mathbf{d}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^T).$$

- *Marginal distribution: If $\tilde{\mathbf{y}} = (y_1, \ldots, y_m)^T \subseteq \mathbf{y}$ is a vector subset of $\mathbf{y}$, then $\tilde{\mathbf{y}}$ is MVN-distributed. In particular, every $y_j \in \mathbf{y} \sim N(\mu_j, \Sigma_{jj})$ is normally distributed.*
- *Conditional distribution: If $\mathbf{u} = (\mathbf{y}_1^T, \mathbf{y}_2^T)^T \sim MVN$ (i.e., breaking a column vector $\mathbf{u}$ into two pieces), then $\mathbf{y}_1^T \mid \mathbf{y}_2^T$ is MVN-distributed.*
- *Independence: If $\Sigma_{ij} = 0$, then y_i and y_j are independent.*
  - *Note this only holds for Normal variables: independence $\implies$ $\mathrm{Cov} = 0$ always holds, but the other direction is generally false (but true for MVN).*

Section 4. Multiple Linear Regression

2.12. Definition: The **multiple linear regression** (MLR) model is given by

$$\boxed{\begin{array}{l} y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_P x_{iP} + \epsilon_i, \quad \epsilon_i \overset{\text{iid}}{\sim} N\left(0, \sigma^2\right) \\ \iff \\ y_i \mid x_i \overset{\text{indep}}{\sim} N\left(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}, \sigma^2\right) \end{array}}$$

- (x_i, y_i): the ith observation, but now we have P covariates instead of just 1.
- The meaning of other symbols remain the same.
- Assume $p < n$, or we have more variates than observations.

2.13. (Cont'd): Equivalently, we can write

$$\boxed{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1P} \\ 1 & x_{21} & x_{22} & \dots & x_{2P} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nP} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_P \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix},}$$

or more compactly,

$$\boxed{\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \text{MVN}(\mathbf{0}, \sigma^2 \mathbf{I}) \iff \mathbf{y} \sim \text{MVN}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I),}$$

where

- $\mathbf{X}$ is the **design matrix**,
- $\boldsymbol{\beta}$ is the **parameter vector**,
- ε is the **error vector**, and
- $\mathbf{y}$ is the **response vector**.

Note $\mathbf{X} \in \mathbb{R}^{n \times (p+1)}$, where each row represents a sample and each column correspond to a covariate.

2.14. Note: How to interpret the regression coefficients:

- β_0 is the mean outcome when all variates are set to 0.
- β_j represents the difference in mean outcome for a 1-unit change in the jth variate x_j, *holding other covariates* fixed.

Section 5. MLR: Least Squares Estimation

2.15. Theorem: *The LS estimators for $\boldsymbol{\beta}$ is given by*

$$\boxed{\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}.}$$

Proof. We wish to minimize the sum of squares:

$$\begin{aligned} S(\boldsymbol{\beta}) &= (\mathbf{y}-\mathbf{X}\boldsymbol{\beta})^T(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\boldsymbol{\beta} - \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{y}^T\mathbf{y} - 2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} && \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y}, \mathbf{y}^T\mathbf{X}\boldsymbol{\beta} \in \mathbb{R} \end{aligned}$$

Taking its derivative with respect to the vector $\boldsymbol{\beta}$, we get

$$\frac{\partial S(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2\mathbf{X}^T\mathbf{y} + (\mathbf{X}^T\mathbf{X} + \mathbf{X}^T\mathbf{X})\boldsymbol{\beta}$$

Note the last term comes from the derivative of the quadratic form

$$\frac{\partial}{\partial \mathbf{y}}(\mathbf{y}^T\mathbf{A}\mathbf{y}) = (\mathbf{A} + \mathbf{A}^T)\mathbf{y}.$$

Now set the derivative to 0,

$$\begin{aligned} -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} &= 0 \\ \left(\mathbf{X}^T\mathbf{X}\right)\boldsymbol{\beta} &= \mathbf{X}^T\mathbf{y} \\ \implies \hat{\boldsymbol{\beta}} &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}. \end{aligned}$$

Note the inverse exists iff $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$ $\mathbf{X}$ has full column rank (i.e., the columns of $\mathbf{X}$ are linearly independent). Thus, we require $n \geq p+1$. □

2.16. Remark: Maximum likelihood gives the same estimators. We omit the derivation.

2.17. Theorem: *The LS estimator $\hat{\boldsymbol{\beta}}$ has the following properties:*

$$\boxed{\begin{aligned} \hat{\boldsymbol{\beta}} &\sim \mathrm{MVN}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}) \\ \hat{\beta}_j &\sim N(\beta_j, \sigma^2[(\mathbf{X}^T\mathbf{X})^{-1}]_{jj}) \end{aligned}}$$

In particular, $\mathbf{V} = (\mathbf{X}^T\mathbf{X})^{-1}$.

Proof.

$$\begin{aligned} \mathbb{E}[\hat{\boldsymbol{\beta}}] &= \mathbb{E}\left[\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}\right] \\ &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbb{E}[\mathbf{y}] && \text{Linearity of } \mathbb{E} \\ &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T(\mathbf{X}\boldsymbol{\beta}) \\ &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\left(\mathbf{X}^T\mathbf{X}\right)\boldsymbol{\beta} \\ &= \boldsymbol{\beta} \end{aligned}$$

$$\begin{aligned}
\operatorname{Var}[\hat{\boldsymbol{\beta}}] &= \operatorname{Var}\left[\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}\right] \\
&= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\operatorname{Var}[\mathbf{y}]\left(\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\right)^T \\
&= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\operatorname{Var}[\mathbf{y}]\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} \\
&= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\left(\sigma^2\mathbf{I}\right)\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} \\
&= \sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} \\
&= \sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1}
\end{aligned}$$

Finally, since $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ is a linear combination of $\mathbf{y} \sim$ MVN, $\hat{\boldsymbol{\beta}}$ is also MVN. The second statement follows from the *marginal distribution* property of MVN. □

2.18. Theorem: *The unbiased estimator of σ^2 is given by*

$$\boxed{\hat{\sigma}^2 = \frac{1}{n-(p+1)}\mathbf{e}^T\mathbf{e}.}$$

Proof. Omitted. □

2.19. Lemma: $(\mathbf{X}^{\mathbf{X}})^{-1}$ *is symmetric.*

Proof. $[(\mathbf{X}^T\mathbf{X})^{-1}]^T = [(\mathbf{X}^T\mathbf{X})^T]^{-1} = (\mathbf{X}^T\mathbf{X})^{-1}$. □

Section 6. MLR: Fitted Values and Residuals

2.20. Definition: Let $\hat{\boldsymbol{\beta}}$ be the LS estimator of $\boldsymbol{\beta}$. The **fitted values** is defined as

$$\begin{aligned}\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} &= \mathbf{X}\left[\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}\right] \\ &= \left[\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\right]\mathbf{y} =: \mathbf{H}\mathbf{y}.\end{aligned}$$

The matrix $\boxed{\mathbf{H} := \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T}$ is called the **Hat matrix**, as applying $\mathbf{H}$ to $\mathbf{y}$ yields $\hat{\mathbf{y}}$ ("adding a hat to $\mathbf{y}$"). You should be familiar with the property $\boxed{\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{H}\mathbf{y}.}$

2.21. Proposition: *The Hat matrix* $\mathbf{H}$ *is symmetric and idempotent (i.e., a projection matrix).*

Proof. $\mathbf{H}\mathbf{H} = \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T = \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T = \mathbf{H}.$ □

2.22. Corollary: $\mathbf{I}-\mathbf{H}$ *is symmetric and idempotent (i.e., a projection matrix).*

Proof. $(\mathbf{I}-\mathbf{H}) = \mathbf{I}^T - \mathbf{H}^T = (\mathbf{I}-\mathbf{H})$. Also, $(\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H}) = \mathbf{I}\mathbf{I} - 2\mathbf{H} + \mathbf{H}\mathbf{H} = \mathbf{I}-\mathbf{H}.$ □

2.23. Proposition: $\boxed{\mathbb{E}[\hat{\mathbf{y}}] = \mathbf{X}\boldsymbol{\beta}, \operatorname{Var}[\hat{\mathbf{y}}] = \sigma^2\mathbf{H}.}$

Proof.

$$\begin{aligned}\mathbb{E}[\hat{\mathbf{y}}] &= \mathbb{E}[\mathbf{H}\mathbf{y}] \\ &= \mathbf{H}\mathbb{E}[\mathbf{y}] \\ &= \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T(\mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{X}\boldsymbol{\beta}\end{aligned} \qquad \begin{aligned}\operatorname{Var}[\hat{\mathbf{y}}] &= \operatorname{Var}[\mathbf{H}\mathbf{y}] \\ &= \mathbf{H}\operatorname{Var}[\mathbf{y}]\mathbf{H}^T \\ &= \mathbf{H}\sigma^2\mathbf{I}\mathbf{H} \\ &= \sigma^2\mathbf{H}\end{aligned}$$

□

2.24. Definition: Define **residuals** as $\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{y} - \mathbf{H}\mathbf{y} = \boxed{(\mathbf{I}-\mathbf{H})\mathbf{y}}.$

2.25. Remark: Note that the sum of residuals is zero:

$$\begin{bmatrix}\sum_{i=1}^n e_i \cdot 1 \\ \sum_{i=1}^n x_{i1}e_i \\ \vdots \\ \sum_{i=1}^n x_{ip}e_i\end{bmatrix} = \mathbf{X}^T\mathbf{e} = \mathbf{X}^T(\mathbf{y}-\mathbf{H}\mathbf{y}) = \mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{y} = \mathbf{0}.$$

2.26. Proposition: $\boxed{\mathbb{E}[\mathbf{e}] = \mathbf{0}, \operatorname{Var}[\mathbf{e}] = \sigma^2(\mathbf{I}-\mathbf{H}).}$

Proof.

$$\begin{aligned}\mathbb{E}[\mathbf{e}] &= \mathbb{E}[(\mathbf{I}-\mathbf{H})\mathbf{y}] \\ &= (\mathbf{I}-\mathbf{H})\mathbb{E}[\mathbf{y}] \\ &= \left(\mathbf{I} - \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\right)(\mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{X}\boldsymbol{\beta} - \mathbf{X}\boldsymbol{\beta} = \mathbf{0}\end{aligned} \qquad \begin{aligned}\operatorname{Var}[\mathbf{e}] &= \operatorname{Var}[(\mathbf{I}-\mathbf{H})\mathbf{y}] \\ &= (\mathbf{I}-\mathbf{H})\operatorname{Var}[\mathbf{y}](\mathbf{I}-\mathbf{H})^T \\ &= \sigma^2(\mathbf{I}-\mathbf{H})\end{aligned}$$

□

2.27. Note: Recall $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ and $\mathbf{e} = (\mathbf{I} - \mathbf{H})\mathbf{y}$ are both linear combinations of $\mathbf{y}$. Since $\mathbf{y}$ is MVN-distributed, the vector obtained by stacking rows of $\hat{\boldsymbol{\beta}}$ on top of the rows of $\mathbf{e}$,

$$\begin{pmatrix} \hat{\boldsymbol{\beta}} \\ \mathbf{e} \end{pmatrix} = \begin{pmatrix} (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\ (\mathbf{I} - \mathbf{H})\mathbf{y} \end{pmatrix} = \begin{pmatrix} (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \\ \mathbf{I} - \mathbf{H} \end{pmatrix} \mathbf{y}$$

is also MVN-distributed. We now explore the relationship between $\hat{\boldsymbol{\beta}}$ and $\mathbf{e}$.

2.28. Theorem:

$$\boxed{\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \mathbf{e} \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{0} \end{bmatrix}, \sigma^2 \begin{bmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1} & \mathbf{0} \\ \mathbf{0} & (\mathbf{I} - \mathbf{H}) \end{bmatrix} \right).}$$

Moreover,

1. $\hat{\boldsymbol{\beta}} \sim \text{MVN}\left(\boldsymbol{\beta}, \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\right)$
2. $\mathbf{e} \sim \text{MVN}\left(\mathbf{0}, \sigma^2(\mathbf{I} - \mathbf{H})\right)$, *and*
3. $\hat{\boldsymbol{\beta}}$ *and* $\mathbf{e}$ *are independent.*

Proof. We already proved Claim 1. For Claim 2 and 3, it suffices to prove that the vector has the claim distribution, as $\boldsymbol{\Sigma}_{22} = \text{Var}[\mathbf{e}]$ and $\boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}_{21} = 0$ indicates variables $\hat{\boldsymbol{\beta}}$ and $\mathbf{e}$ are independent.

$$\begin{aligned} \mathbb{E}[\mathbf{e}] &= \mathbb{E}[(\mathbf{I} - \mathbf{H})\mathbf{y}] \\ &= (\mathbf{I} - \mathbf{H})E[\mathbf{y}] \\ &= (\mathbf{I} - \mathbf{H})\mathbf{X}\hat{\beta} \\ &= \mathbf{X}\hat{\beta} - \mathbf{H}\mathbf{X}\hat{\beta} \\ &= \mathbf{X}\hat{\beta} - \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\hat{\beta} \\ &= \mathbf{X}\hat{\beta} - \mathbf{X}\hat{\beta} \\ &= \mathbf{0} \end{aligned}$$

$$\begin{aligned} \text{Var}\begin{bmatrix} \hat{\beta} \\ \mathbf{e} \end{bmatrix} &= \text{Var}\left[\begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T \\ (\mathbf{I} - \mathbf{H}) \end{pmatrix} \mathbf{y}\right] \\ &= \begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T \\ (\mathbf{I} - \mathbf{H}) \end{pmatrix} \text{Var}[\mathbf{y}] \begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}X^T \\ (\mathbf{I} - \mathbf{H}) \end{pmatrix}^T \\ &= \sigma^2 \begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T \\ (\mathbf{I} - \mathbf{H}) \end{pmatrix} \begin{pmatrix} \left(\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\right)^T & (\mathbf{I} - \mathbf{H})^T \end{pmatrix} && \text{Var}[\mathbf{y}] = \sigma^2\mathbf{I} \\ &= \sigma^2 \begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T \\ (\mathbf{I} - \mathbf{H}) \end{pmatrix} \begin{pmatrix} \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} & (\mathbf{I} - \mathbf{H}) \end{pmatrix} \\ &= \sigma^2 \begin{pmatrix} \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} & \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T(\mathbf{I} - \mathbf{H}) \\ (\mathbf{I} - \mathbf{H})\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} & (\mathbf{I} - \mathbf{H})(\mathbf{I} - \mathbf{H}) \end{pmatrix} \\ &= \sigma^2 \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \end{aligned}$$

Now

$$\mathbf{A} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}$$

$$\begin{aligned}\mathbf{B} &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T(\mathbf{I}-\mathbf{H})\\ &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T - \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\left(\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\right)\\ &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T - \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T = \mathbf{0} = \mathbf{C}^T\end{aligned}$$

$$\begin{aligned}\mathbf{D} &= (\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H})^T\\ &= \left(\mathbf{I}\mathbf{I}^T - \mathbf{I}\mathbf{H}^T - \mathbf{H}\mathbf{I}^T + \mathbf{H}\mathbf{H}^T\right)\\ &= (\mathbf{I}-2\mathbf{H}-\mathbf{H}) = (\mathbf{I}-\mathbf{H})\end{aligned}$$

□

Section 7. MLR: Deriving t-Statistic*

2.29. Remark (Review on eigen-decomposition)**:** Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ with n linearly independent eigenvectors q_i, $1 \le i \le n$. Then $\mathbf{A}$ can be factorized as $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$ where $\mathbf{Q} \in \mathbb{R}^{n\times n}$, whose ith column is the eigenvector q_i of $\mathbf{A}$, and $\mathbf{\Lambda}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues, $\Lambda_{ii} = \lambda_i$. Only diagonalizable matrices can be factorized in this way.

2.30. Note: So far, we have proved that

$$\hat{\beta} \sim N\left(\beta, \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\right) \Longrightarrow \hat{\beta}_j \sim N\left(\beta_j, \sigma^2 V_{jj}\right).$$

If we can show that

1. $\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e} \sim \chi^2_{n-(p+1)}$, and
2. it is independent of $\hat{\boldsymbol{\beta}}$,

then we obtain the following t-statistic, which can be used for constructing confidence intervals and hypothesis testing. Note we did something similar for SLR but we didn't give a mathematical proof back then.

$$\frac{\frac{\hat{\beta}_j-\beta_j}{\sqrt{\sigma^2 V_{jj}}}}{\sqrt{\left(\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e}\right)/(n-(p+1))}} = \frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 V_{jj}}} \sim t_{n-(p+1)}.$$

Intuitively, we have $n-(p+1)$ degrees of freedom because we have n data points and we are trying to estimate $p+1$ regression parameters. We now show the math behind this.

2.31. (Cont'd): The second condition is easy. Since $\mathbf{e}$ is independent of $\hat{\boldsymbol{\beta}}$, $\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e}$ as a function of $\mathbf{e}$ is also independent of $\hat{\boldsymbol{\beta}}$. Now for the first condition, recall that $\mathbf{e} = (\mathbf{I}-\mathbf{H})\mathbf{y}$. Consider the eigen-decomposition $\mathbf{I}-\mathbf{H} = \mathbf{\Gamma}^T\mathbf{D}\mathbf{\Gamma}$ where $\mathbf{\Gamma}^{-1} = \mathbf{\Gamma}^T$ and

$$\mathbf{D} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{bmatrix}$$

is the diagonal matrix whose diagonal contains the eigenvalues of $(\mathbf{I}-\mathbf{H})$. Define $\tilde{\mathbf{e}} = \mathbf{\Gamma}\mathbf{e}$. Then

$$\begin{aligned}
\mathbb{E}[\tilde{\mathbf{e}}] &= \mathbb{E}[\mathbf{\Gamma}\mathbf{e}] = \mathbf{\Gamma}\mathbb{E}[\mathbf{e}] = \mathbf{0} \\
\mathrm{Var}[\tilde{\mathbf{e}}] &= \mathrm{Var}[\mathbf{\Gamma}\mathbf{e}] \\
&= \mathbf{\Gamma}\,\mathrm{Var}[\mathbf{e}]\mathbf{\Gamma}^T && \mathrm{Var}[\mathbf{A}\mathbf{e}] = \mathbf{A}\mathrm{Var}[\mathbf{e}]\mathbf{A}^T \\
&= \sigma^2\mathbf{\Gamma}(\mathbf{I}-\mathbf{H})\mathbf{\Gamma}^T && \mathrm{Var}[\mathbf{e}] = \mathbf{I}-\mathbf{H} \\
&= \sigma^2\mathbf{\Gamma}\left(\mathbf{\Gamma}^T\mathbf{D}\mathbf{\Gamma}\right)\mathbf{\Gamma}^T \\
&= \sigma^2\mathbf{D}
\end{aligned}$$

Thus, $\tilde{\mathbf{e}} \sim \mathrm{MVN}(\mathbf{0}, \sigma^2\mathbf{D})$ as $\mathbf{e} \sim \mathrm{MVN}$, which implies

$$\tilde{e}_i \overset{\text{indep}}{\sim} N(0, \sigma^2[\mathbf{D}]_{ii}) = N(0, \sigma^2\lambda_i^2).$$

2.32. Remark (Review on χ^2 Distributions)**:** For standard normal rvs $Z_i \overset{\text{iid}}{\sim} N(0,1)$,

$$X = \sum_{i=1}^{n} Z_i^2 \sim \chi_n^2.$$

2.33. (Cont'd): Next,

$$\tilde{\mathbf{e}}^T\tilde{\mathbf{e}} = (\mathbf{\Gamma e})^T(\mathbf{\Gamma e}) = \mathbf{e}^T\mathbf{\Gamma}^T\mathbf{\Gamma e} = \mathbf{e}^T\mathbf{e},$$

so we can write

$$\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e} = \frac{1}{\sigma^2}\tilde{\mathbf{e}}^T\tilde{\mathbf{e}} = \sum_{i=1}^{n}\left(\frac{\tilde{e}_i}{\sigma}\right)^2 = \sum_{i=1}^{n} Z_i^2, \qquad Z_i \overset{\text{indep}}{\sim} N(0,\lambda_i^2).$$

Thus, $\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e}$ is a sum of squared independent normally distributed rvs. To show

$$\frac{1}{\sigma^2}\mathbf{e}^T\mathbf{e} \sim \chi^2_{(n-(p+1))},$$

we need to show that $n-(p+1)$ of the eigenvalues λ_j's are equal to 1, and all others are equal to 0. (Indeed, if $\lambda_j = 0$, then $Z_j \sim N(0,0)$ becomes a constant.) We know that $(\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H}) = \mathbf{I}-\mathbf{H}$. This gives

$$\begin{aligned}(\mathbf{I}-\mathbf{H})(\mathbf{I}-\mathbf{H}) &= \mathbf{I}-\mathbf{H}\\ (\mathbf{\Gamma}^T\mathbf{D\Gamma})(\mathbf{\Gamma}^T\mathbf{D\Gamma}) &= (\mathbf{\Gamma}^T\mathbf{D\Gamma})\\ \mathbf{\Gamma}^T\mathbf{DD\Gamma} &= \mathbf{\Gamma}^T\mathbf{D\Gamma},\end{aligned}$$

i.e., $\mathbf{DD} = \mathbf{D}$ and thus $\lambda_j^2 = \lambda_j$. Thus all λ_j are either 0 or 1. Next,

$$\begin{aligned}\sum_j \lambda_j = \operatorname{tr}(\mathbf{D}) &= \operatorname{tr}\left(\mathbf{D\Gamma\Gamma}^T\right) && \text{trace is similarity-invariant}\\ &= \operatorname{tr}\left(\mathbf{\Gamma}^T\mathbf{D\Gamma}\right) && \text{invariant under cyclic permutation}\\ &= \operatorname{tr}(\mathbf{I}-\mathbf{H}) && \\ &= \operatorname{tr}(\mathbf{I}) - \operatorname{tr}(\mathbf{H}) && \text{trace is linear}\\ &= n - \operatorname{tr}(\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T) && \\ &= n - \operatorname{tr}(\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}) && \text{invariant under cyclic permutation}\\ &= n - \operatorname{tr}(\mathbf{I}_{p+1}) && \mathbf{X} \in \mathbb{R}^{n\times(p+1)} \implies \mathbf{X}^T\mathbf{X} \in \mathbb{R}^{(p+1)(p+1)}\\ &= n-(p+1)\end{aligned}$$

This concludes our proof.

2.34. Note: This entire section is optional. The only thing you need to remember is that

$$\boxed{\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 V_{jj}}} \sim t_{n-(p+1)}.}$$

Moreover, the standard error of $\hat{\beta}_j$ is given by

$$\boxed{\mathrm{SE}(\hat{\beta}_j) = \hat{\sigma}\sqrt{V_{jj}}.}$$

Section 8. MLR: Hypothesis Testing

2.35. Note: Suppose we want to test a null hypothesis $H_0 : \beta_j = \theta_0$ against some alternative hypothesis $H_1 : \beta_j \neq \theta_0$. Our goal is to characterize how much evidence we have against H_0, or more intuitively, how *extreme* are our data relative to H_0. Under H_0 (i.e., if H_0 holds), then

$$T := \frac{\hat{\beta}_j - \theta_0}{\hat{\sigma}/\sqrt{V_{jj}}} \sim t_{n-p-1}.$$

Below we discuss two approaches for hypothesis testing.

2.36. (Cont'd): First, we can compute the p-value and compare it against α.

1. Given observed value

$$T_{\text{obs}} := \frac{\hat{\beta}_j - \theta_0}{\hat{\sigma}/\sqrt{V_{jj}}} \sim t_{n-p-1},$$

2. Compute the p-value $p = \Pr(|T| \geq |T_{\text{obs}}|) = 2\Pr(T \geq T_{\text{obs}})$ given by

```
p <- pq(T_obs, df = n-p-1, lower.tail=FALSE).
```

3. If $p < \alpha$, reject H_0 (at α).

2.37. (Cont'd): Alternatively, we can compute the quantile, known as the **critical value**, of the test statistic T that gives a p-value of α, then compare our observed value with this threshold.

1. Given observed value

$$T_{\text{obs}} := \frac{\hat{\beta}_j - \theta_0}{\hat{\sigma}/\sqrt{V_{jj}}} \sim t_{n-p-1},$$

2. Compute the threshold by

```
q <- qt(p = alpha/2, df=n-p-1).
```

3. If $|T_{\text{obs}}| < t_{n-p-1,1-\alpha/2} = \texttt{q}$, reject H_0 (at α).

2.38. Theorem: *A* $(100-\alpha)\%$ *CI for* β_j *is*

$$\boxed{\hat{\beta}_j \pm t_{n-p-1,1-\alpha/2}\hat{\sigma}\sqrt{V_{jj}}.}$$

Proof. Omitted. □

2.39. Note: We can never guarantee that any single CI contains the true value. However, as we repeatedly construct CIs, about $(100-\alpha)\%$ of them will contain the true value.

Section 9. MLR: Estimating Mean Response

2.40. For an arbitrary vector of covariates $\mathbf{x}_0 = [1, x_{01}, x_{02}, \ldots, x_{0p}]$, the mean response is

$$\mu_0 = \mathbb{E}[\mathbf{y}_0 \mid \mathbf{x}_0] = \mathbf{x}_0\boldsymbol{\beta}.$$

We can estimate this as $\hat{\mu}_0 = \mathbf{x}_0\hat{\boldsymbol{\beta}}$. We now look at the properties of this estimator.

2.41. Proposition:

$$\boxed{\begin{aligned} \mathbb{E}[\hat{\mu}_0] &= \mathbf{x}_0\boldsymbol{\beta} \\ \operatorname{Var}[\hat{\mu}_0] &= \sigma^2\mathbf{x}_0\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T \end{aligned}}$$

Proof.

$$\begin{aligned} \mathbb{E}[\hat{\mu}_0] &= \mathbb{E}[\mathbf{x}_0\hat{\boldsymbol{\beta}}] \\ &= \mathbf{x}_0\mathbb{E}[\hat{\boldsymbol{\beta}}] \\ &= \mathbf{x}_0\boldsymbol{\beta} \end{aligned}$$

$$\begin{aligned} \operatorname{Var}[\hat{\mu}_0] &= \operatorname{Var}\left(\mathbf{x}_0\hat{\boldsymbol{\beta}}\right) \\ &= \mathbf{x}_0\operatorname{Var}(\hat{\boldsymbol{\beta}})\mathbf{x}_0^T \\ &= \mathbf{x}_0\sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T \\ &= \sigma^2\mathbf{x}_0\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T \end{aligned}$$

□

2.42. Note: By the same logic as before,

$$\begin{aligned} \frac{\hat{\mu}_0 - \mu_0}{\sigma\sqrt{\mathbf{x}_0\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T}} &\sim N(0,1), \\ \frac{\hat{\mu}_0 - \mu_0}{\hat{\sigma}\sqrt{\mathbf{x}_0\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T}} &\sim t_{n-p-1}, \end{aligned}$$

and a $100(1-\alpha)\%$ CI is given by

$$\boxed{\hat{\mu}_0 \pm t_{n-p-1,1-\frac{\alpha}{2}}\hat{\sigma}\sqrt{\mathbf{x}_0\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{x}_0^T}.}$$

Section 10. MLR: Prediction

2.43. Note: For a new response

$$y_{\text{new}} = \mathbf{x}_{\text{new}}\, \boldsymbol{\beta} + \boldsymbol{\epsilon}_{\text{new}}\ ,$$

our prediction is

$$\hat{y}_{\text{new}} = \mathbf{x}_{\text{new}}\, \hat{\boldsymbol{\beta}}.$$

2.44. Proposition:

$$\boxed{\begin{aligned} \mathbb{E}[\hat{y}_{\text{new}}] &= \mathbf{x}_{\text{new}}\boldsymbol{\beta} + \boldsymbol{\epsilon}_{new} \\ \text{Var}[\hat{y}_{\text{new}}\ ] &= \sigma^2 \mathbf{x}_{\text{new}}\ \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \mathbf{x}_{\text{new}}^T \end{aligned}}$$

Proof.

$$\begin{aligned} \mathbb{E}\left[\hat{y}_{\text{new}}\ \right] &= \mathbb{E}\left[\mathbf{x}_{\text{new}}\ \hat{\boldsymbol{\beta}}\right] \\ &= \mathbf{x}_{\text{new}}\ \mathbb{E}[\hat{\boldsymbol{\beta}}] \\ &= \mathbf{x}_{\text{new}}\ \boldsymbol{\beta} \end{aligned}$$

$$\begin{aligned} \text{Var}\left[\hat{y}_{\text{new}}\ \right] &= \text{Var}\left(\mathbf{x}_{\text{new}}\ \hat{\boldsymbol{\beta}}\right) \\ &= \mathbf{x}_{\text{new}}\ \ \text{Var}(\hat{\boldsymbol{\beta}})\mathbf{x}_{\text{new}}^T \\ &= \mathbf{x}_{\text{new}}\ \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \mathbf{x}_{\text{new}}^T \\ &= \sigma^2 \mathbf{x}_{\text{new}}\ \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \mathbf{x}_{\text{new}}^T \end{aligned}$$

□

2.45. Note: Since y_{new} and $\hat{y}_{\text{new}}$ are independent and normally-distributed, we have

$$\frac{y_{\text{new}}\ - \hat{y}_{\text{new}}}{\sigma\sqrt{1 + \mathbf{x}_{\text{new}}\ (\mathbf{X}^T\mathbf{X})^{-1} \mathbf{x}_{\text{new}}^T}} \sim N(0,1),$$

$$\frac{y_{\text{new}}\ - \hat{y}_{\text{new}}}{\hat{\sigma}\sqrt{1 + \mathbf{x}_{\text{new}}\ (\mathbf{X}^T\mathbf{X})^{-1} \mathbf{x}_{\text{new}}^T}} \sim t_{n-p-1}$$

Thus, a $100(1-\alpha)\%$ prediction interval for y_{new} is

$$\boxed{\hat{y}_{\text{new}}\ \pm t_{n-p-1,1-\alpha/2}\hat{\sigma}\sqrt{1 + \mathbf{x}_{\text{new}}\ \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \mathbf{x}_{\text{new}}^T}\ .}$$

Section 11. MLR: Categorical Covariates

2.46. Let `weight` be continuous and `fishpart` be categorical with four possible values:

- none (N)
- muscle tissue only (M)
- muscle tissue and sometimes whole fish (MW)
- whole fish (W)

Let `MeHg`(the concentration of methyl mercury extracted from hair sample) be the (continuous) response variable. For simplicity, let us ignore `weight` for now and only model the relationship between `fishpart` and `MeHg`. How should we encode `fishpart`? We will see that the way we encode the categorical covariates imposes assumptions on our model. In particular, it affects how we interpret the model parameters.

2.47. Naively, we could use numbers $0, 1, 2, 3$ to encode $\mathtt{N}, \mathtt{M}, \mathtt{MW}, \mathtt{W}$ (so that $\mathtt{fishpart}_i \in \{0, 1, 2, 3\}$ for each i) and use

$$\mathtt{MeHg}_i = \beta_0 + \beta_1 \mathtt{fishpart}_i + \varepsilon, \qquad \varepsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2).$$

This model implicitly assumes that the difference between each consecutive factor of `fishpart` is the same. Some assumptions we made include:

- the mean difference of `MeHg` between people of group i and people of group $i+1$ is always β_1;
- the mean difference of `MeHg` between people of group i and people of group $i+2$ is $2\beta_1$;
- the mean difference of `MeHg` between people of group 3 and people of group 0 is $3\beta_1$, etc.

It is easy to see that if we had used other numbers (instead of 0 to 3) to encode the groups, then the model assumptions will be different.

2.48. We often don't want to make assumption about the relative differences between categories. A more flexible alternative is to use **indicator functions** and write

$$\begin{aligned}\mathtt{MeHg}_i \sim \gamma_{\mathtt{N}} \cdot \mathbf{1}\left[\mathtt{fishpart}_i = \mathtt{N}\right] &+ \gamma_{\mathtt{M}} \cdot \mathbf{1}\left[\mathtt{fishpart}_i = \mathtt{M}\right] \\ &+ \gamma_{\mathtt{MW}} \cdot \mathbf{1}\left[\mathtt{fishpart}_i = \mathtt{MW}\right] \\ &+ \gamma_{\mathtt{W}} \cdot \mathbf{1}\left[\mathtt{fishpart}_i = \mathtt{W}\right] + \epsilon_{\mathrm{i}}, \quad \epsilon \overset{\text{iid}}{\sim} N(0, \sigma^2).\end{aligned}$$

We essentially fitted four models based on `fishpart` with same variance but different mean; no assumption about relative differences between categories are made here:

$$\begin{aligned}\mathtt{MeHg} \mid \{\mathtt{fishpart=N}\} &\sim N\left(\gamma_{\mathtt{N}}, \sigma^2\right) \\ \mathtt{MeHg} \mid \{\mathtt{fishpart=M}\} &\sim N\left(\gamma_{\mathtt{M}}, \sigma^2\right) \\ \mathtt{MeHg} \mid \{\mathtt{fishpart=MW}\} &\sim N\left(\gamma_{\mathtt{MW}}, \sigma^2\right) \\ \mathtt{MeHg} \mid \{\mathtt{fishpart=W}\} &\sim N\left(\gamma_{\mathtt{W}}, \sigma^2\right)\end{aligned}$$

Another way to interpret this is that we are fitting four models with different intercepts and 0 slope (as `fishpart` is the only covariate here), i.e., they are horizontal lines at $y = \gamma_X$ with $X \in \{\mathtt{N}, \mathtt{M}, \mathtt{MW}, \mathtt{W}\}$.

2.49. We can replace the first term $\gamma_{\texttt{N}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{N}\right]$ with a β_0 and replace all γ's with β's. The resulting model will look more familiar to us:

$$\begin{aligned}\texttt{MeHg}_i \sim \beta_0 &+ \beta_{\texttt{M}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{M}\right]\\ &+ \beta_{\texttt{MW}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{MW}\right]\\ &+ \beta_{\texttt{W}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{W}\right] + \epsilon_i, \quad \epsilon \overset{\text{iid}}{\sim} N(0, \sigma^2)\end{aligned}$$

The relationship between γ's and β's are given below:

- $\gamma_{\texttt{N}} = \beta_0$;
- $\gamma_{\texttt{M}} = \beta_0 + \beta_{\texttt{M}}$;
- $\gamma_{\texttt{MW}} = \beta_0 + \beta_{\texttt{MW}}$;
- $\gamma_{\texttt{W}} = \beta_0 + \gamma_{\texttt{W}}$.

and

- $\beta_0 = \gamma_{\texttt{N}}$;
- $\beta_{\texttt{N}} = \gamma_{\texttt{M}} - \gamma_{\texttt{N}}$;
- $\beta_{\texttt{MW}} = \gamma_{\texttt{MW}} - \gamma_{\texttt{N}}$;
- $\beta_{\texttt{W}} = \gamma_{\texttt{W}} - \gamma_{\texttt{N}}$;

Interpretation of γ's and β's:

- γ_X represents the mean `MeHg` for people of group X;
- β_0 represents the mean `MeHg` for people of group N, known as the **reference group**;
- β_X represents the difference of the mean `MeHg` between group X and the reference group.

2.50. Let us add the continuous covariate `weight`back. We can encode a regression model where expected `MeHg` is *linear* in `weight` for each level of `fishpart`, with common slope but different intercepts as follows:

$$\begin{aligned}\texttt{MeHg}_i \sim \gamma_1 \texttt{weight} &+ \gamma_{\texttt{N}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{N}\right]\\ &+ \gamma_{\texttt{M}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{M}\right]\\ &+ \gamma_{\texttt{MW}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{MW}\right]\\ &+ \gamma_{\texttt{W}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{W}\right] + \epsilon_{\text{i}}, \quad \epsilon \overset{\text{iid}}{\sim} N(0, \sigma^2)\end{aligned}$$

Interpretation of the parameters:

- γ_1 is the mean difference of `MeHg` for one unit of change in `weight`, holding `fishpart` constant.

$$\gamma_1 = \mathbb{E}[y \mid \texttt{weight} = w^*, \texttt{fishpart} = X] - \mathbb{E}[y \mid \texttt{weight} = w^* - 1, \texttt{fishpart} = X]$$

- γ_X is the mean `MeHg` of people of group X ($\texttt{fishpart}_i = X$), holding `weight` at 0.

$$\gamma_X = \mathbb{E}[y \mid \texttt{weight} = 0, \texttt{fishpart} = X].$$

This model consists of four submodels with different intercepts (γ_X's) but a common slope (γ_1).

2.51. The corresponding β model is given below:

$$\begin{aligned} \texttt{MeHg}_i \sim \beta_0 &+ \beta_1 \texttt{weight} \\ &+ \beta_{\texttt{M}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{M}\right] \\ &+ \beta_{\texttt{MW}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{MW}\right] \\ &+ \beta_{\texttt{W}} \cdot \mathbf{1}\left[\texttt{fishpart}_i = \texttt{W}\right] + \epsilon_i, \quad \epsilon \overset{\text{iid}}{\sim} N(0, \sigma^2) \end{aligned}$$

Interpretation of the parameters:

- β_0 is the mean outcome of the reference group, holding `weight` at 0:
$$\beta_0 = \mathbb{E}[y \mid \texttt{weight} = 0, \texttt{fishpart} = \texttt{N}].$$
- β_1 is the mean difference of `MeHg` for one unit change in `weight`, holding `fishpart` constant:
$$\beta_1 = \mathbb{E}[y \mid \texttt{weight} = w^*, \texttt{fishpart} = X] - \mathbb{E}[y \mid \texttt{weight} = w^* - 1, \texttt{fishpart} = X].$$
- β_X is the mean difference of `MeHg` between group X and the reference group, holding `weight` constant:
$$\beta_X = \mathbb{E}[y \mid \texttt{weight} = w^*, \texttt{fishpart} = X] - \mathbb{E}[y \mid \texttt{weight} = w^*, \texttt{fishpart} = N].$$

This model consists of four submodels with different intercepts (β_0 or $\beta_0 + \beta_X$) and a common slope (β_1). The actual graph will be the same as the γ-model.

Section 12. MLR: Hypotheses Testing (Categorical Covariates)

2.52. Suppose we want to test whether the average MeHg varies by fishpart adjusted for weight. There are two equivalent null hypotheses:

1. $\gamma_N = \gamma_M = \gamma_{MW} = \gamma_W$.
2. $\beta_M = \beta_{MW} = \beta_W = 0$.

The second is simpler for testing, so we'll proceed with the β-model from here on out.

2.53. To compare one group to the reference group:

$$\frac{\hat{\beta}_M - 0}{\mathrm{SE}(\hat{\beta}_M)} \sim N(0,1)$$

To compare two non-reference groups:

$$\frac{\hat{\beta}_M - \hat{\beta}_{NW}}{\mathrm{SE}(\hat{\beta}_M - \hat{\beta}_{MW})} \sim N(0,1)$$

where

$$\begin{aligned}\mathrm{Var}(\hat{\beta}_{\mathrm{M}} - \hat{\beta}_{\mathrm{MW}}) &= \mathrm{Var}(\hat{\beta}_{\mathrm{M}}) + \mathrm{Var}(\hat{\beta}_{\mathrm{MW}}) - 2\,\mathrm{Cov}(\hat{\beta}_{\mathrm{M}}, \hat{\beta}_{\mathrm{MW}}) \\ &= \sigma^2\,(V_{3,3} + V_{4,4} - 2V_{3,4})\end{aligned}$$

Don't forget to estimate σ^2 by $\hat{\sigma}^2$ and plug in $V = (X^T X)^{-1}$ as the covariance matrix

2.54. Suppose now we want to compare more than two groups. For example, does mean MeHg vary by fishpart, adjusted for weight? The null is given by

$$H_0 : \beta_* = (\beta_M, \beta_{MW}, \beta_W)^T = \mathbf{0}.$$

Recall that

$$\hat{\beta} \sim N(\beta, \sigma^2(X^T X)^{-1}) \implies \hat{\beta}_* \sim N(\beta, \sigma^* V_*)$$

where V_* is the corresponding sub-matrix.

2.55. Theorem (Cholesky Decomposition)**:** *Any covariance matrix V can be uniquely decomposed as $V = LL^T$ where L is a lower triangular matrix with non-negative entries $L_{ii} \geq 0$ on the diagonal. When V is positive-definite, then $L_{ii} > 0$.*

2.56. Let L be a lower-triangular matrix such that $\sigma^2 V_* = LL^T$ and define $Z = L^{-1}(\hat{\beta}_* - \beta_*)$. Note that $Z \sim N(0, I)$:

$$\begin{aligned}\mathbb{E}[Z] &= L^{-1}\mathbb{E}[\hat{\beta}_*] - L^{-1}\mathbb{E}[\beta_*] = L^{-1}\beta_* = L^{-1}\beta_* = 0 \\ \mathrm{Var}[Z] &= \mathrm{Var}[L^{-1}(\hat{\beta}_* - \beta_*)] \\ &= \mathrm{Var}[L^{-1}\hat{\beta}_*] \\ &= L^{-1}\mathrm{Var}(\hat{\beta}_*)(L^{-1})^T = L^{-1}\sigma^2 V_*(L^{-1})^T = L^{-1}LL^T(L^{-1})^T = I\end{aligned}$$

Let q be the dimension of β_*. Consider the sum of q squared standard normals:

$$\begin{aligned}\sum_{j=1}^{q} Z_j^2 &= Z^T Z \\ &= (\hat{\beta}_* - \beta_*)^T (L^{-1})^T L^{-1} (\hat{\beta}_* - \beta_*) \\ &= (\hat{\beta}_* - \beta_*)^T (LL^T)^{-1} (\hat{\beta}_* - \beta_*) \\ &= \frac{1}{\sigma^2}(\hat{\beta}_* - \beta_*)^T (V_*)^{-1} (\hat{\beta}_* - \beta_*). \quad (LL^T)^{-1} = (\sigma^2 V_*)^{-1}\end{aligned}$$

Thus, under H_0, we have that

$$\frac{1}{\sigma^2}(\hat{\beta}_*)^T (V_*)^{-1} (\hat{\beta}_*) = \sum_{j}^{q} Z_j^2 \sim \chi_q^2$$

and this is independent of (shown previously)

$$\frac{n-(p+1)}{\sigma^2}\hat{\sigma}^2 \sim \chi^2_{n-(p+1)},$$

Define an F-statistic:

$$F = \frac{\frac{1}{\sigma^2}(\hat{\beta}_*)^T (V_*)^{-1} (\hat{\beta}_*)/q}{\frac{n-(p+1)}{\sigma^2}\hat{\sigma}^2/(n-(p+1))} = \frac{(\hat{\beta}_*)^T (V_*)^{-1} (\hat{\beta}_*)}{q\hat{\sigma}^2}$$

obtained by dividing each random variable by its degree of freedom. Under H_0,

$$F = \frac{(\hat{\beta}_*)^T (V_*)^{-1} (\hat{\beta}_*)}{q\hat{\sigma}^2} \sim F(q, n-(p+1))$$

2.57. Definition (F-distribution)**:** Let $X_1 \sim \chi^2_{\nu_1}$ and $X_2 \sim \chi^2_{\nu_2}$ be independent. Then

$$W = \frac{x_1/\nu_1}{x_2/\nu_2}$$

has an F-distribution:

$$\begin{aligned} W &\sim F(\nu_1, \nu_2) \\ f(w) &= \frac{\Gamma((\nu_1+\nu_2)/2)}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} \left(\nu_1^{\nu_1} \nu_2^{\nu_2} \frac{w^{\nu_1 - 2}}{(\nu_2 + \nu_1 w)^{(\nu_1+\nu_2)}} \right)^{1/2}\end{aligned}$$

2.58. We can test H_0 by comparing F to the corresponding F distribution.

```
pf(F_obs, df1=3, df2=n-p-1, lower.tail=FALSE)
```

Section 13. MLR: Intersections and Non-Linearities

2.59. Consider the model from last section:

$$\texttt{MeHg}_i \sim \beta_0 + \beta_1 \texttt{weight}_i + \beta_{\texttt{M}}\texttt{M}_i + \beta_{\texttt{MW}}\texttt{MW}_i + \beta_{\texttt{W}}\texttt{W}_i + \epsilon_i, \quad \epsilon \overset{\text{iid}}{\sim} N\left(0, \sigma^2\right)$$

where $X_i = \mathbf{1}[\texttt{fishpart}_i = X]$ denotes the corresponding indicator function. Recall this implies common slope for weight for any value of `fishpart` (i.e., parallel lines with different intercepts). What if we want different intercepts and different slopes?

2.60. Consider the following model.

$$\begin{aligned}\texttt{MeHg}_i \sim{}& \beta_0 + \beta_1 \texttt{weight}_i + \beta_{\texttt{M}}\texttt{M}_i + \beta_{\texttt{MW}}\texttt{MW}_i + \beta_{\texttt{W}}\texttt{W}_i \\ &+ \beta_{1\texttt{M}}\texttt{weight}_i\texttt{M}_i + \beta_{1\texttt{MW}}\texttt{weight}_i\texttt{MW}_i + \beta_{1\texttt{W}}\texttt{weight}_i\texttt{W}_i + \epsilon_i, \quad \epsilon \overset{\text{iid}}{\sim} N\left(0, \sigma^2\right)\end{aligned}$$

We added three columns to our design matrix. More specifically, the design matrix looks as follows:

- The first column consists of just 1s.
- The second column contains weights, real numbers.
- The next three columns correspond to $\texttt{M}_i, \texttt{MW}_i, \texttt{W}_i$, so either 0 or 1.
- The last three columns are the products of $X_i \cdot \texttt{weight}_i$. If $X_i = 0$ then the entry is 0; otherwise the entry is $\texttt{weight}_i$.

2.61. To see that this model gives different mean and different intercepts, observe that if $\texttt{fishpart}_i = \texttt{N}$, the mean outcome is given by

$$\mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i, \texttt{N}_i = 1] = \beta_0 + \beta_1 \texttt{weight}_i,$$

so the mean is linear in $\texttt{weight}_i$ with intercept β_0. For $\texttt{fishpart}_i = \texttt{MW}$, the mean outcome is

$$\begin{aligned}\mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i, \texttt{MW}_i = 1] &= \beta_0 + \beta_1 \texttt{weight}_i + \beta_{1\texttt{MW}}\texttt{weight}_i + \beta_{\texttt{MW}} \\ &= (\beta_0 + \beta_{\texttt{MW}}) + (\beta_1 + \beta_{1\texttt{MW}})\texttt{weight}_i.\end{aligned}$$

The mean is still linear in $\texttt{weight}_i$, but with a different slope and a different intercept. Terms like $\texttt{weight}_i\texttt{MW}_i$, where different covariates are multiplied together, are called **interaction terms**. They are preferable here as they allow different slopes.

2.62. Note: Time for the interpretation of the parameters. The parameter β_1 is the mean difference in `MeHg` for one unit change of `weight`, provided that $\texttt{fishpart}_i = \texttt{N}$

$$\begin{aligned}\beta_1 &= \mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i = x^* + 1, \texttt{N}_i = 1] - \mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i = x^*, \texttt{N}_i = 1] \\ &= (\beta_0 + \beta_1(x^* + 1)) - (\beta_0 + \beta_1 x^*).\end{aligned}$$

$\beta_{1\texttt{MW}} + \beta_1$ is the mean difference in `MeHg` for one unit change of `weight`, given that $\texttt{fishpart}_i = \texttt{MW}$.

$$\begin{aligned}\beta_1 &= \mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i = x^* + 1, \texttt{MW}_i = 1] - \mathbb{E}[\texttt{MeHg}_i \mid \texttt{weight}_i = x^*, \texttt{MW}_i = 1] \\ &= (\beta_0 + \beta_{MW} + \beta_1(x^* + 1) + \beta_{1\texttt{MW}}(x^* + 1)) - (\beta_0 + \beta_1 x^* + \beta_1 x^* + \beta_{1\texttt{MW}} x^*).\end{aligned}$$

Thus, $\beta_{1\texttt{MW}}$ is the difference between "mean difference in `MeHg` for one unit change of `weight`, provided that $\texttt{fishpart}_i = \texttt{MW}$" and "mean difference in `MeHg` for one unit change of `weight`, provided that $\texttt{fishpart}_i = \texttt{N}$". It is the increase of the *slope* compared to the slope of the reference group.

2.63. Note (Interactions of continuous covariates)**:** Let x_{i1} and x_{i2} be continuous covariates and consider the following model:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i1} x_{i2} + \epsilon_i$$

We can bruteforce this by observing that

$$\beta_1 = \mathbb{E}[y_i \mid x_{i2} = 0, x_{i1} = x^* + 1] - \mathbb{E}[y_i \mid x_{i2} = 0, x_{i1} = x^*],$$

i.e., it is the average change of outcome for one unit change of x_{i1}, holding $x_{i2} = 0$. This is not very intuitive. A better way to interpret this is to observe that

- at every level of x_2, the conditional mean outcome is linear in x_1;
- at every level of x_2, the intercept and slope of x_1 are different.

Since the change in mean outcome due to one unit change in x_1 varies with x_2, it's better to fix a set of x_{i2}'s and then report the corresponding β_3 as the average change of outcome for one unit change of x_{i1}.

2.64. Note (More Flexible Models)**:** Sometimes a simple linear model does not fit the data well. One way to make the model more flexible is to include a quadratic term for x:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i.$$

Note here the change in mean outcome for a one unit change in x_i varies with x_i. To test whether the quadratic model is more appropriate than the simple linear one, the null hypothesis is $H_0 : \beta_2 = 0$. Beyond polynomial terms, linear regression can be specified flexibly:

$$y_i = \sum_{j=1}^{p} \beta_j f_j(x_i) + \epsilon_i$$

where $f_j(\cdot)$ are arbitrary functions of x_i. However, there is a tradeoff between *fit* and *interpretability.*

2.65. Note (Hierarchical Principle)**:**

- If there is a higher order interaction term, include main effects (and lower order interaction terms), i.e.:
  - If including $x_1 \cdot x_2$, include also x_1 and x_2 (main effects).
  - If including $x_1 \cdot x_2 \cdot x_3$, include also $x_1 \cdot x_2$ and $x_2 \cdot x_3, x_1 \cdot x_3$, and main effects.
- If there is a higher order polynomial term, include main effects and lower order terms
  - If including x^3, include also x^2 and x.

Otherwise can have unexpected interpretations/implications.

2.66. Example: Consider the model $y_i = \beta_0 + \beta_2 x_i^2 + \varepsilon_i$. Now suppose we shift the exposure by some fixed amount b, e.g., center the x_i to have mean 0 (so b = $\bar{x}$):

$$\begin{aligned} y_i &= \beta_0 + \beta_2 (x_i - b)^2 + \epsilon_i \\ &= \beta_0 + \beta_2 \left(x_i^2 - 2x_i b + b^2\right) + \epsilon_i \\ &= \left(\beta_0 + b^2 \beta_2\right) + (-2b\beta_2)\, x_i + \beta_2 x_i^2 + \epsilon_i \end{aligned}$$

Suddenly, there is now a linear term, simply because of a shift!

Section 14. Analysis of Variance and R^2

2.67. Motivation: Recall the **sample variance** is given by

$$s^2 = \frac{1}{n-1}\sum(y_i - \bar{y})^2.$$

Suppose we wish to quantify how much of the variability in the outcome $\mathbf{y}$ is explained by our model. That is, we want to decompose the sum of squares $\sum(y_i - \bar{y})^2$ into two parts, one for the variance we can explain with our model and one for the variance we cannot explain.

2.68. Definition (ANOVA Decomposition)**:** Define the following terms:

- **Total sum of squares**, SSTotal, quantifies how much the data points y_i vary around their mean $\bar{y}$.

$$\text{SSTotal} = \sum_{i=1}^{n}(y_i - \bar{y})^2 = (\mathbf{y} - \bar{y}\mathbf{1})^T(\mathbf{y} - \bar{y}\mathbf{1}) = \mathbf{y}^T\mathbf{y} - n\bar{y}^2.$$

- **Regression sum of squares**, SSReg, quantifies how far the estimated regression model $\hat{y}_i$ is from the horizontal "no relationship line", the sample mean $\bar{y}$.

$$\text{SSReg} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 = (\mathbf{Hy} - \bar{y}\mathbf{1})^T(\mathbf{Hy} - \bar{y}\mathbf{1}) = \mathbf{y}^T\mathbf{Hy} - n\bar{y}^2.$$

- **Residual sum of squares**, SSRes, quantifies how much the data points y_i vary around the regression estimates $\hat{y}_i$.

$$\text{SSRes} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = (\mathbf{y} - \mathbf{Hy})^T(\mathbf{y} - \mathbf{Hy}) = \mathbf{y}^T(\mathbf{I} - \mathbf{H})\mathbf{y}.$$

2.69. Theorem (ANOVA Decomposition)**:** SSTotal = SSReg + SSRes.

Proof. Observe that

$$\begin{aligned}
\text{SSTotal} &= \sum_{i=1}^{n}(y_i - \bar{y})^2 \\
&= \sum_{i=1}^{n}([y_i - \hat{y}_i] + [\hat{y}_i - \bar{y}])^2 \\
&= \sum_{i=1}^{n}[y_i - \hat{y}_i]^2 + \sum_{i=1}^{n}[\hat{y}_i - \bar{y}]^2 + 2\sum_{i=1}^{n}[y_i - \hat{y}_i][\hat{y}_i - \bar{y}] \\
&= \text{SSRes} + \text{SSReg} + 0
\end{aligned}$$

where we used the fact that

$$\sum_{i=1}^{n}[y_i - \hat{y}_i][\hat{y}_i - \bar{y}] = \sum_{i=1}^{n}e_i[\hat{y}_i - \bar{y}] = \mathbf{e}^T[\hat{\mathbf{y}} - \bar{y}\mathbf{1}] = \mathbf{e}^T\mathbf{X}\hat{\boldsymbol{\beta}} - \bar{y}\mathbf{e}^T\mathbf{1} = 0 - 0 = 0.$$

as $\mathbf{e}^T\mathbf{X} = \mathbf{e}^T\mathbf{1} = \mathbf{0}$. □

2.70. Definition: The **coefficient of decomposition** defined as

$$R^2 = \frac{\text{SSReg}}{\text{SSTotal}} = 1 - \frac{\text{SSRes}}{\text{SSTotal}} \in [0,1]$$

is the proportion of the variance in the outcome that is explained by our regression model.

2.71. Note:

- Since R^2 is a proportion, it is always a scalar between 0 and 1.
- If $R^2 = 1$, then $\sum(y_i - \bar{y})^2 = \sum(\hat{y}_i - \bar{y})^2$, so all data points fall on our regression line and the model perfectly captures all variability of the data.
- If $R^2 = 0$, then $\sum(\hat{y}_i - \bar{y})^2 = 0$, so $\hat{y}_i = \bar{y}$ for every i, i.e., our regression model is just the line of mean $\bar{y}$ and no variance is explained by our model.
- Thus, a higher R^2 indicates that more variability in the outcome is explained by our model.

2.72. Remark: In SLR, $R^2 = r^2$ where r is the coefficient of correlation.

2.73. Note (F-Test for Model Significance)**:** Suppose we want to test the significance of the regression model, i.e., is there any relationship between the outcome and *at least one* covariate? Consider the following hypotheses:[1]

$$\begin{aligned} H_0 &: \beta_1 = \cdots = \beta_p = 0 \\ H_1 &: \exists i \in \{1, \ldots, p\} : \beta_j \neq 0. \end{aligned}$$

We can conduct an F-test with the SS decomposition. Under the null,

$$\begin{aligned} \frac{\text{SSReg}}{\sigma^2} &\sim \chi^2_p \\ \frac{\text{SSRes}}{\sigma^2} &\sim \chi^2_{n-(p+1)} \end{aligned}$$

and they're independent, so we can define the F-statistic

$$F = \frac{\text{SSReg}/p}{\text{SSRes}/n - (p+1)} \sim F_{p,n-(p+1)}.$$

Reject null if p-value $< \alpha$. If we reject H_0, we conclude that at least one of the regression coefficients is non-zero. Otherwise, we don't have enough evidence to conclude that none of β_j is important.

2.74. Note (ANOVA Table)**:** We can summarize everything into a table:

Source	SS	df	MS	F
Regression	SSReg $= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$	p	MSReg $= \frac{\text{SSReg}}{p}$	$\frac{\text{MSReg}}{\text{MSRes}} = \frac{\text{SSReg}}{p} \Big/ \frac{\text{SSRes}}{n-(p+1)}$
Residuals	SSRes $= \sum_{i=1}^n (y_i - \hat{y})^2$	$n - (p+1)$	MSRes $= \frac{\text{SSRes}}{n-(p+1)}$	
Total	SSTotal $= \sum_{i=1}^n (y_i - \bar{y})^2$	$n - 1$		

[1] Note that we are not imposing any condition on the intercept β_0.

2.75. Note (F-Test for a Subset of Covariates)**:** Suppose we want to test $\beta_j = 0$ for q of the p covariates. Intuitively, we are testing whether these q covariates are not very useful in our model:

$$\begin{aligned} H_0 &: \beta_{k_1} = \cdots = \beta_{k_q} = 0 \\ H_1 &: \exists i \in \{k_1, \ldots, k_q\} : \beta_{k_i} \neq 0. \end{aligned}$$

Suppose we fit the full model as before and additionally fit a *reduced model* under the null. The *additional variation* explained by the identified q covariates

$$\text{SSReg(Full)} - \text{SSReg(Reduced)}$$

has q degrees of freedom. Under H_0, we thus have

$$\frac{(\text{SSReg(Full)} - \text{SSReg(Reduced)})/q}{\text{SSRes}/n - (p+1)} \sim F_{q,n-(p+1)}$$

Note that F-Test for Model Significance can be viewed as a special case of this where we are testing the significance of all p covariates.

2.76. Note (F-Test for General Linear Hypothesis)**:** We can use the same infrastructure to test a broader class of null hypothesis, called **general linear hypotheses**, all of the form

$$\begin{aligned} H_0 &: \mathbf{C}\boldsymbol{\beta} = \mathbf{0} \\ H_1 &: \mathbf{C}\boldsymbol{\beta} \neq \mathbf{0} \end{aligned}$$

Here $\mathbf{C} \in \mathbb{R}^{\ell \times (p+1)}$ is a matrix of rank r representing the hypotheses. In particular, ℓ denotes the number of linear constraints. For example, given a model

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \varepsilon_i,$$

the matrices corresponding to the null hypotheses are given by

$$\begin{aligned} H_0 : \beta_1 = \beta_2 = 0 &\iff \mathbf{C} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \\ H_0 : \beta_1 = \beta_2 &\iff \mathbf{C} = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 \end{bmatrix} \end{aligned}$$

Fit the full model and the reduced model (the model under $\mathbf{C}\boldsymbol{\beta} = \mathbf{0}$) and then construct F statistic:

$$\frac{(\text{SSReg(Full)} - \text{SSReg(Reduced)})/r}{\text{SSRes}/n - (p+1)} \sim F_{r,n-(p+1)}$$

where $r = \text{rank}(C)$.

Section 15. Multicollinearity and Variance Inflation Factor

2.77. Motivation: Multicollinearity is a phenomenon in which one covariate in a MLR model can be linearly predicted from the others with a substantial degree of accuracy. In this situation, the coefficient estimates of the MLR model may change erratically in response to small changes in the model or the data. Multicollinearity does not reduce the predictive power or reliability of the model as a whole, at least within the sample data set; it only affects calculations regarding individual predictors. That is, a multivariate regression model with collinear predictors can indicate how well the entire bundle of predictors predicts the outcome variable, but it may not give valid results about any individual predictor, or about which predictors are redundant with respect to others.

2.78. Definition: **Collinearity** is a linear association between two covariates. Two variables are **perfectly collinear** if there is an exact linear relationship between them. **Multicollinearity** refers to a situation in which more than two covariates in a MLR model are highly linearly related.

2.79. Note (Perfect Multicollinearity in OLS)**:** Recall OLS requires *no multicollinearity*, i.e., there cannot exist an exact (non-stochastic) linear relation among the covariates, because in that case the design matrix $\mathbf{X}$ has less than full rank, and therefore the moment matrix $\mathbf{X}^T\mathbf{X}$ cannot be inverted. Under these circumstances, for a general linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, the OLS estimators $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ does not exist.

2.80. Note (VIF)**:** To detect pairwise collinearity, we may plot the correlation matrix and look for correlation values which are close to one. It's much hard to detect multicollinearity. One intuitive thing to do is to try to predict one covariate x_j using the rest with a MLR model, i.e., let x_j be the true outcome and consider the model

$$x_j = \mathbf{X}_{-j}\boldsymbol{\alpha} + \boldsymbol{\epsilon}^*$$

where $\mathbf{X}_{-j}$ denotes the matrix obtained by removing the column corresponding to x_j from $\mathbf{X}$ and $\boldsymbol{\alpha}, \boldsymbol{\epsilon}^*$ play the role of $\boldsymbol{\beta}, \boldsymbol{\varepsilon}$, respectively. The fitted values are

$$\hat{x}_j = \mathbf{X}_{-j}\hat{\boldsymbol{\alpha}}$$

where $\hat{\boldsymbol{\alpha}}$ is estimator of $\boldsymbol{\alpha}$. Recall in SLR, $r_{yx}^2 = R^2$. It turns out that in MLR, $r_{y,\hat{y}}^2 = R^2$. Therefore, the coefficient of correlation between the true y and the fitted $\hat{y}$ is exactly R^2. In particular, this is true in the regression of x_j on $\mathbf{X}_{-j}$. Thus, we could examine $r_{x_j,\hat{x}_j}^2$ which is equal to the R_j^2 for the regression of x_j on X_{-j}. This motivates the following definition.

2.81. Definition: Let R_j the coefficient of correlation for the regression on x_j using other covariates. The **variance inflation factor** (VIF) defined by

$$\mathrm{VIF}_j := \frac{1}{1 - R_j^2}$$

quantifies the severity of multicollinearity in a regression analysis. It provides an index that measures how much the variance of an estimated regression coefficient is increased due to collinearity, i.e., how much it is increased relative to the ideal case in which all covariates are uncorrelated (i.e., the columns of X are orthogonal).

2.82. Note: Consider the MLR $y = \beta_0 + \beta_1 X_1 + \cdots + \beta_k X_k + \varepsilon$. It turns out that the variance of the estimator of β_j can be expressed as

$$\mathrm{Var}(\hat{\beta}_j) = \frac{\hat{\sigma}^2}{\sum(x_{ij} - \bar{x}_j)^2} \times \frac{1}{1 - R_j^2}.$$

We make the following observations:

- σ^2: greater scatter in the data around the regression surface leads to proportionately more variance in the coefficient estimates.
- $\sum(x_{ij} - \bar{x}_j)^2$: greater variability in a particular covariate leads to proportionately less variance in the corresponding coefficient estimate.

The remaining term, $1/(1 - R_j^2)$, is the VIF. It reflects all other factors that influence the uncertainty in the coefficient estimates. The VIF equals 1 when the vector X_j is orthogonal to every other column of the design matrix. By contrast, the VIF is greater than 1 when the vector X_j is not orthogonal to all columns of the design matrix for the regression of X_j on the other covariates. Finally, note that the VIF is invariant to the scaling of the variables.