

# Math 6040/7260 Linear Models

Mon/Wed/Fri 9:00am - 9:50am

Instructor: Dr. Xiang Ji, xji4@tulane.edu

## 1 Lecture 1: Jan 18

### Today

- Introduction
- Introduce yourself
- Course logistics

### What is this course about?

The term “linear models” describes a wide class of methods for the statistical analysis of multivariate data. The underlying theory is grounded in linear algebra and multivariate statistics, but applications range from biological research to public policy. The objective of this course is to provide a solid introduction to both the theory and practice of linear models, combining mathematical concepts with realistic examples.

### Prerequisite

- **Must:** Introduction to Probability (Math 3070/6070), Mathematical Statistics (Math 3080/6080)
- **Good to have:** Scientific Computation II

### A hierarchy of linear models

- The linear mean model:

$$\underset{n \times 1}{\mathbf{y}} = \underset{n \times p}{\mathbf{X}} \underset{p \times 1}{\boldsymbol{\beta}} + \underset{n \times 1}{\boldsymbol{\epsilon}}$$

where  $\mathbf{E}(\boldsymbol{\epsilon}) = \mathbf{0}$ . Only assumption is that errors have mean 0.

- Gauss-Markov model:

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

where  $\mathbf{E}(\boldsymbol{\epsilon}) = \mathbf{0}$  and  $\mathbf{Var}(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}$ . Uncorrelated errors with constant variance.

- Aitken model or general linear model:

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

where  $\mathbf{E}(\boldsymbol{\epsilon}) = \mathbf{0}$  and  $\mathbf{Var}(\boldsymbol{\epsilon}) = \sigma^2 \mathbf{V}$ .  $\mathbf{V}$  is fixed and known.

- Variance components models:  $\mathbf{y} \sim N(\mathbf{X}\beta, \sigma_1^2\mathbf{V}_1 + \sigma_2^2\mathbf{V}_2 + \dots + \sigma_r^2\mathbf{V}_r)$  with  $\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_r$  known.
- General mixed linear Model:

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$

where  $\mathbf{E}(\epsilon) = \mathbf{0}$  and  $\mathbf{Var}(\epsilon) = \Sigma(\theta)$ .

- Generalized linear models (GLMs). Logistic regression, probit regression, log-linear model (Poisson regression), ... Note the difference from the general linear model. GLMs are generalization of the *concept* of linear models. They are covered in Math 7360 - Data Analysis class (<https://tulane-math-7360-2021.github.io/>).

## Syllabus

Check course website frequently for updates and announcements.

<https://tulane-math-7260-2023.github.io/>

## HW submission

Through Github with demo on Friday class.

## Presentations

Let me know your pick by the end of Friday (01/20/2023).

## Last year (spring 2022) comments

### 1. Experience in this course

- I really enjoyed this class.
- The lecture is dry. Expect Dr. Ji to read through the lecture notes until someone asks a question. Also, having a background in statistics gives context to the lecture notes.

*Response:* I did emphasize on pre-requisite last year, but it still seemed not enough.

- I think this course was well laid out. Even though I did take it as a graduation requirement, I ended up enjoying the course. I also think the work load is manageable and professor Xi does provide all the tools necessary to succeed in the course. It can be overwhelming at first but with a little time and effort you can get the hang of the material.

*Response:* Mind the typos, students.

### 2. Strong aspects of this course

- Professor Ji is a great professor.

- Dr. Ji provides an inhuman amount of course material to help supplement learning, it was extremely helpful to have labs (answered and unanswered) as well as homework keys posted.

*Response:* There will be labs again.

- Notes are very structured and the professor is nice.
- The strongest aspect of this course is the homework. They are a great way to interact with and learn the material. The problems can seem challenging, but are doable with a little effort. Also, he publishes the keys afterword so you can check your work and see what the reasoning behind the answer is. This coupled with the lab sessions are a great way to prepare for the exams.

3. There will be an internal mid-term-ish evaluation for this course. Will remember to go over them.

## Last last year (spring 2021) comments

### 1. Experience in this course

- Overall, I had a pretty good experience in this course. It moved quickly, but that is expected from this level of course. Sometimes it was hard to stay engaged with the lectures and to really absorb the course material. Because the lectures moved so fast, I really appreciated how Professor made the full notes available at the time of the lecture. I would have liked if there were a few more examples with the notes, as sometimes the homework felt disjoint from the notes.

*Response:* I will try to move slower this semester. I will start lab sessions earlier too.

- The professor is an extremely intelligent, kind, and understanding professor. He prioritizes in making sure that we understand the material and seeing how the material can be applied. His lecture notes were a godsend because the texts could be a bit ambiguous at times but he elucidated the material in such a comprehensible manner.

*Response:* I will try to fix the left-over typos.

- Mentioned in class from other students/internal evaluation, conveying the mathematical concepts through the presentation is not a good idea to follow the class in real-time. Prepared presentation can give rise to a distraction on what we have been going over.

*Response:* I am still delivering this class in hybrid-mode. I found the presentations fit online teaching better. I think the difficulty might be caused by (1) fast moving lecture (2) I only realized the need of reviewing basic concepts of probability almost a quarter into the semester...

- I found the setup of the course not very engaging. Additionally, many of the class notes came directly from the additional sources with no additional information or

explanation, which I found to be not very helpful.

*Response:* I actually like them. I was the guinea pig to test them.

- Easily help us to understand the main course, and the notes and details are great.

*Response:* There will be notes.

- Moves very quickly and can be hard to keep up with. Sometimes instructions are unclear.

*Response:* I will try to slow down.

- Both the instructor and the TA were helpful. It was hard to follow along in class though.

*Response:* We don't have TA this time. Make use of the office hour. And I have to say, it needs effort to ace in this class.

## 2. Strong aspects of this course

- Having the lecture notes and labs available was very helpful. Professor was also always very nice and accommodating, and willing to meet with me when I needed help. He also always responded to student feedback, if we asked for an extra day or two on the homework or something like that.

*Response:* Here is an example of correctly using the office hours.

- His lecture notes and the lab sessions.

*Response:* They will be there again.

- Lab session is necessarily required to this class. A lot of computations in the class would be done by computer due to the complexity, and students are expected to handle with the computer programming properly at a desired level. The course can be an introduction to the statistical computation, which does not exist in the mathematics department.

*Response:* Hmm, there is a course Math 7360 Data Analysis that focuses more on the computational side.

- I appreciated the homework reviews in class and felt these helped clarify the material.

*Response:* Of course, the reviews will be there again. The purpose of the course is for you to learn.

- Grading was easy which made up for the rigor.

*Response:* Don't rely on this...

- Really appreciate that Professor Xiang made such a neat and tidy notes for us. It is really helpful for me to review. And notes have a great interaction with us, Professor Xiang also leaves some questions to help us think about the logic behind.

*Response:* Well, Xiang is my first name. Please call me Prof. X.

- Prof. Xiang was highly organized and wanted his students to understand the course content more than he made them worry about grades. I learned a lot

about Linear Models and feel confident applying the course content professionally and academically. I wish most of the Math department had his teaching style and implemented his course documents and organization structure. Prof. Xiang made the course content in class digestible and if I needed to review the material I could easily find it through his course notes and textbook. I wish I could say the same about my other courses.

*Response:* Hmm, I like Prof. X. better.

- I really appreciated the emphasis on learning. It allowed for most students to take it at the pace that was good for them.

*Response:* Please don't let your score rely on this comment.

3. There will be an internal mid-term-ish evaluation for this course. Will remember to go over them.

## 2 Lecture 2:Jan 20

### Last time

- Introduction
- Course logistics

### Today

- Reply to the “Presentation Dates” thread on Canvas by the end of today.
- Git

### What is git?

Git is currently the most popular system for version control according to [Google Trend](#). Git was initially designed and developed by [Linus Torvalds](#) in 2005 for Linux kernel development. Git is the British English slang for unpleasant person.

### Why using git?

- [GitHub](#) is becoming a de facto central repository for open source development.
- **Advertise** yourself through GitHub (e.g., host a free personal webpage on GitHub).
- a skill that employers look for (according to [this AmStat article](#)).

### Git workflow

Figure 2.1 shows its basic workflow.

### What do I need to use Git?

- A **Git server** enabling multi-person collaboration through a centralized repository.
- A **Git client** on your own machine.
  - Linux: Git client program is shipped with many Linux distributions, e.g., Ubuntu and CentOS. If not, install using a package manager, e.g., `yum install git` on CentOS.
  - Mac: follow instructions at <https://www.atlassian.com/git/tutorials/install-git>.
  - Windows: Git for Windows at <https://gitforwindows.org> (GUI) aka Git Bash.
- Do **not** totally rely on GUI or IDE. Learn to use Git on command line, which is needed for cluster and cloud computing.



Figure 2.1

## Git survival commands

- `git pull` synchronize local Git directory with remote repository.
- Modify files in local working directory.
- `git add FILES` add snapshots to staging area
- `git commit -m "message"` store snapshots permanently to (**local**) Git repository
- `git push` push commits to remote repository.

## Git basic usage

Working with your local copy.

- `git pull` : update local Git repository with remote repository (fetch + merge).
- `git log FILENAME` : display the current status of working directory.
- `git diff` : show differences (by default difference from the most recent commit).
- `git add file1 file2 ...` : add file(s) to the staging area.

- `git commit` : commit changes in staging area to Git directory.
- `git push` : publish commits in local Git repository to remote repository.
- `git reset --soft HEAD 1` : undo the last commit.
- `git checkout FILENAME` : go back to the last commit, discarding all changes made.
- `git rm FILENAME` : remove files from git control.

## Git demonstration

Show how to create a private git repository for HW and Exam submissions.

On [GitHub](#)

- Obtain [student developer pack](#).
- Create a private repository `math-6040-2023-spring` (please substitute 6040 by 7260 if you are taking the graduate level). Add `xji3` as your collaborators with write permission ([instruction](#)).

On your local machine:

- clone the repository: please refer to [this webpage](#) with instructions for your operating system.
- enter the folder: `cd math-6040-2023-spring`.
- after finishing the rest of the questions, save your file inside your git repository folder `math-6040-2023-spring` with name `hw1.pdf` (for example). Please make it human-readable.
- now using git commands to stage this change: `git add hw1.pdf`
- commit: `git commit -m "hw1 submission"` (remember to replace the quotation mark)
- push to remote server: `git push`
- tag version hw1: `git tag hw1` and push: `git push --tags`.

Take a look at the tags on GitHub ([instructions](#)).

When submitting your hw, please email your instructor ([xji4@tulane.edu](mailto:xji4@tulane.edu)) a link to your tag ([instructions](#)).



### 3 Lecture 3:Jan 23

Last time

- Git

Today

- HW1 posted
- Linear algebra: vector and vector space, rank of a matrix
- Column space and Nullspace (JM Appendix A)

Notations

$$\underset{n \times 1}{\mathbf{y}} = \underset{n \times p}{\mathbf{X}} \underset{p \times 1}{\boldsymbol{\beta}} + \underset{n \times 1}{\boldsymbol{\epsilon}}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

- All vectors are column vector
- Write dimensions underneath as in  $\underset{n \times p}{\mathbf{X}}$  or as  $\mathbf{X} \in \mathbb{R}^{n \times p}$
- Bold upper-case letters for Matrices. Bold lower-case letters for Vectors.

Vector and vector space

(from JM Appendix A)

- A set of vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n$  are *linearly dependent* if there exist coefficients  $c_j$  for  $j = 1, 2, \dots, n$  such that  $\sum_{j=1}^n c_j \mathbf{x}_j = \mathbf{0}$  and  $\|\mathbf{c}\|_2 = \sum_{j=1}^n c_j^2 > 0$ . They are *linearly independent* if  $\sum_{j=1}^n c_j \mathbf{x}_j = \mathbf{0}$  implies (i.e.  $\implies$ )  $c_j = 0$  for all  $j$ .
- Two vectors are *orthogonal* to each other, written  $\mathbf{x} \perp \mathbf{y}$ , if their inner product is 0, that is  $\mathbf{x}^T \mathbf{y} = \mathbf{y}^T \mathbf{x} = \sum_j x_j y_j = 0$ .
- A set of vectors  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}$  are mutually orthogonal iff (i.e.  $\iff$ )  $\mathbf{x}^{(i)T} \mathbf{x}^{(j)} = 0$  for  $\forall i \neq j$ .
- The most common set of vectors that are mutually orthogonal are the *elementary* vectors  $\mathbf{e}^{(1)}, \mathbf{e}^{(2)}, \dots, \mathbf{e}^{(n)}$ , which are all zero, except for one element equal to 1, so that  $\mathbf{e}_i^{(i)} = 1$  and  $\mathbf{e}_j^{(i)} = 0, \forall j \neq i$ .

- A *vector space*  $\mathcal{S}$  is a set of vectors that are closed under addition and scalar multiplication, that is
  - if  $\mathbf{x}^{(1)}$  and  $\mathbf{x}^{(2)}$  are in  $\mathcal{S}$ , then  $c_1\mathbf{x}^{(1)} + c_2\mathbf{x}^{(2)}$  is in  $\mathcal{S}$ .
- A vector space  $\mathcal{S}$  is *generated* or *spanned* by a set of vectors  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}$ , written as  $\mathcal{S} = \text{span}\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}\}$ , if any vector  $\mathbf{x}$  in the vector space is a linear combination of  $\mathbf{x}_i, i = 1, 2, \dots, n$ .
- A set of linearly independent vectors that generate or span a space  $\mathcal{S}$  is called a *basis* of  $\mathcal{S}$ .

### Example A.1

Let

$$\mathbf{x}^{(1)} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \mathbf{x}^{(2)} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}, \text{ and } \mathbf{x}^{(3)} = \begin{bmatrix} -3 \\ -1 \\ 1 \\ 3 \end{bmatrix}.$$

Then  $\mathbf{x}^{(1)}$  and  $\mathbf{x}^{(2)}$  are linearly independent, but  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}$ , and  $\mathbf{x}^{(3)}$  are linearly dependent since  $5\mathbf{x}^{(1)} - 2\mathbf{x}^{(2)} + \mathbf{x}^{(3)} = \mathbf{0}$

## Rank

Some matrix concepts arise from viewing columns or rows of the matrix as vectors. Assume  $\mathbf{A} \in \mathbb{R}^{m \times n}$ .

- $\text{rank}(\mathbf{A})$  is the maximum number of linearly independent rows or columns of a matrix.
- $\text{rank}(\mathbf{A}) \leq \min\{m, n\}$ .
- A matrix is *full rank* if  $\text{rank}(\mathbf{A}) = \min\{m, n\}$ . It is *full row rank* if  $\text{rank}(\mathbf{A}) = m$ . It is *full column rank* if  $\text{rank}(\mathbf{A}) = n$ .
- a square matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is *singular* if  $\text{rank}(\mathbf{A}) < n$  and *non-singular* if  $\text{rank}(\mathbf{A}) = n$ .
- $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}^T) = \text{rank}(\mathbf{A}^T \mathbf{A}) = \text{rank}(\mathbf{A} \mathbf{A}^T)$ . (Show this in HW.)
- $\text{rank}(\mathbf{A} \mathbf{B}) \leq \min\{\text{rank}(\mathbf{A}), \text{rank}(\mathbf{B})\}$ . (Hint: Columns of  $\mathbf{A} \mathbf{B}$  are spanned by columns of  $\mathbf{A}$  and rows of  $\mathbf{A} \mathbf{B}$  are spanned by rows of  $\mathbf{B}$ .)
- if  $\mathbf{A} \mathbf{x} = \mathbf{0}_m$  for some  $\mathbf{x} \neq \mathbf{0}_n$ , then  $\text{rank}(\mathbf{A}) \leq n - 1$ .

## Column space

*Definition:* The column space of a matrix, denoted by  $\mathcal{C}(\mathbf{A})$  is the vector space spanned by the columns of the matrix, that is,

$$\mathcal{C}(\mathbf{A}) = \{\mathbf{x} : \text{there exists a vector } \mathbf{c} \text{ such that } \mathbf{x} = \mathbf{A} \mathbf{c}\}.$$

This means that if  $\mathbf{x} \in \mathcal{C}(\mathbf{A})$ , we can find coefficients  $c_j$  such that

$$\mathbf{x} = \sum_j c_j \mathbf{a}^{(j)}$$

where  $\mathbf{a}^{(j)} = \mathbf{A}_{\cdot j}$  denotes the  $j^{\text{th}}$  column of matrix  $\mathbf{A}$ .

- The column space of a matrix consists of all vectors formed by multiplying that matrix by any vector.
- The number of basis vectors for  $\mathcal{C}(\mathbf{A})$  is then the number of linearly independent columns of the matrix  $\mathbf{A}$ , and so,  $\dim(\mathcal{C}(\mathbf{A})) = \text{rank}(\mathbf{A})$ .
- The dimension of a space is the number of vectors in its basis.

### Example A.2

Let  $\mathbf{A} = \begin{bmatrix} 1 & 1 & -3 \\ 1 & 2 & -1 \\ 1 & 3 & 1 \\ 1 & 4 & 3 \end{bmatrix}$  and  $\mathbf{c} = \begin{bmatrix} 5 \\ 4 \\ 3 \end{bmatrix}$ . Show that  $\mathbf{Ac}$  is a linear combination of columns in  $\mathbf{A}$ .

*solution:*

$$\mathbf{Ac} = \begin{bmatrix} 1 \times 5 + 1 \times 4 + (-3) \times 3 \\ 1 \times 5 + 2 \times 4 + (-1) \times 3 \\ 1 \times 5 + 3 \times 4 + 1 \times 3 \\ 1 \times 5 + 4 \times 4 + 3 \times 3 \end{bmatrix} = \begin{bmatrix} 0 \\ 10 \\ 20 \\ 30 \end{bmatrix}.$$

You could recognize that

$$\mathbf{Ac} = 5 \times \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + 4 \times \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} + 3 \times \begin{bmatrix} -3 \\ -1 \\ 1 \\ 3 \end{bmatrix} = 5\mathbf{a}^{(1)} + 4\mathbf{a}^{(2)} + 3\mathbf{a}^{(3)} = \begin{bmatrix} 0 \\ 10 \\ 20 \\ 30 \end{bmatrix}.$$

### Result A.1

$$\text{rank}(\mathbf{AB}) \leq \min(\text{rank}(\mathbf{A}), \text{rank}(\mathbf{B})).$$

*proof:* Each column of  $\mathbf{AB}$  is a linear combination of columns of  $\mathbf{A}$  (i.e.  $(\mathbf{AB})_{\cdot j} = \mathbf{A}\mathbf{b}^{(j)}$ ), so the number of linearly independent columns of  $\mathbf{AB}$  cannot be greater than that of  $\mathbf{A}$ . Similarly,  $\text{rank}(\mathbf{AB}) = \text{rank}(\mathbf{B}^T \mathbf{A}^T)$ , the same argument gives  $\text{rank}(\mathbf{B}^T)$  as an upper bound.

### Result A.2

- (a) If  $\mathbf{A} = \mathbf{BC}$ , then  $\mathcal{C}(\mathbf{A}) \subseteq \mathcal{C}(\mathbf{B})$ .
- (b) If  $\mathcal{C}(\mathbf{A}) \subseteq \mathcal{C}(\mathbf{B})$ , then there exists a matrix  $\mathbf{C}$  such that  $\mathbf{A} = \mathbf{BC}$ .

*proof:* For (a), any vector  $\mathbf{x} \in \mathcal{C}(\mathbf{A})$  can be written as  $\mathbf{x} = \mathbf{Ad} = \mathbf{B}(\mathbf{Cd})$ .

For (b),  $\mathbf{A}_{\cdot j} \in \mathcal{C}(\mathbf{B})$ , so that there exists a vector  $\mathbf{c}^{(j)}$  such that  $\mathbf{A}_{\cdot j} = \mathbf{B}\mathbf{c}^{(j)}$ . The matrix  $\mathbf{C} = (\mathbf{c}^{(1)}, \mathbf{c}^{(2)}, \dots, \mathbf{c}^{(n)})$  satisfies that  $\mathbf{A} = \mathbf{BC}$ .

## 4 Lecture 4: Jan 25

### Last time

- Linear algebra: vector and vector space, rank of a matrix
- Column space (JM Appendix A)

### Today

- Nullspace
- Probability review

### Null space

*Definition:* The null space of a matrix, denoted by  $\mathcal{N}(\mathbf{A})$ , is  $\mathcal{N}(\mathbf{A}) = \{\mathbf{y} : \mathbf{A}\mathbf{y} = \mathbf{0}\}$ .

#### Result A.3

If  $\mathbf{A}$  has full-column rank, then  $\mathcal{N}(\mathbf{A}) = \{\mathbf{0}\}$ .

*proof:* Matrix  $\mathbf{A}$  has full-column rank means its columns are linearly independent, which means that  $\mathbf{A}\mathbf{c} = \mathbf{0}$  implies  $\mathbf{c} = \mathbf{0}$ .

#### Theorem A.1

Assume  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , then  $\dim(\mathcal{C}(\mathbf{A})) = r$  and  $\dim(\mathcal{N}(\mathbf{A})) = n - r$ , where  $r = \text{rank}(\mathbf{A})$ .

See JM Appendix Theorem A.1 for the proof.

*proof:* Denote  $\dim(\mathcal{N}(\mathbf{A}))$  by  $k$ , to be determined, and construct a set of basis vectors for  $\mathcal{N}(\mathbf{A}) : \{\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \dots, \mathbf{u}^{(k)}\}$ , so that  $\mathbf{A}\mathbf{u}^{(i)} = \mathbf{0}$ , for  $i = 1, 2, \dots, k$ . Now, construct a basis for  $\mathbb{R}^n$  by adding the vectors  $\{\mathbf{u}^{(k+1)}, \dots, \mathbf{u}^{(n)}\}$ , which are not in  $\mathcal{N}(\mathbf{A})$ . Clearly,  $\mathbf{A}\mathbf{u}^{(i)} \in \mathcal{C}(\mathbf{A})$  for  $i = k+1, \dots, n$ , and so the span of these vectors form a subspace of  $\mathcal{C}(\mathbf{A})$ . These vectors  $\{\mathbf{A}\mathbf{u}^{(i)}, i = k+1, \dots, n\}$  are also linearly independent from the following argument: suppose  $\sum_{i=k+1}^n c_i \mathbf{A}\mathbf{u}^{(i)} = \mathbf{0}$ ; then  $\sum_{i=k+1}^n c_i \mathbf{A}\mathbf{u}^{(i)} = \mathbf{A} [\sum_{i=k+1}^n c_i \mathbf{u}^{(i)}] = \mathbf{0}$ , and hence  $\sum_{i=k+1}^n c_i \mathbf{u}^{(i)}$  is a vector in  $\mathcal{N}(\mathbf{A})$ . Therefore, there exist  $b_i$  such that  $\sum_{i=k+1}^n c_i \mathbf{u}^{(i)} = \sum_{i=1}^k b_i \mathbf{u}^{(i)}$ , or  $\sum_{i=1}^k b_i \mathbf{u}^{(i)} - \sum_{i=k+1}^n c_i \mathbf{u}^{(i)} = \mathbf{0}$ . Since  $\{\mathbf{u}^{(i)}\}$  form a basis for  $\mathbb{R}^n$ ,  $c_i$  must all be zero. Therefore  $\mathbf{A}\mathbf{u}^{(i)}, i = k+1, \dots, n$  are linearly independent. At this point, since  $\text{span}\{\mathbf{A}\mathbf{u}^{(k+1)}, \dots, \mathbf{A}\mathbf{u}^{(n)}\} \subseteq \mathcal{C}(\mathbf{A})$ ,  $\dim(\mathcal{C}(\mathbf{A}))$  is at least  $n - k$ . Suppose there is a vector  $\mathbf{y}$  that is in  $\mathcal{C}(\mathbf{A})$ , but not in the span; then there exists  $\mathbf{u}^{(n+1)}$  so that  $\mathbf{y} = \mathbf{A}\mathbf{u}^{(n+1)}$  and  $\mathbf{u}^{(n+1)}$  is linearly independent of  $\{\mathbf{u}^{(k+1)}, \dots, \mathbf{u}^{(n)}\}$  (and clearly not in  $\mathcal{N}(\mathbf{A})$ ), making  $n+1$  linearly independent vectors in  $\mathbb{R}^n$ . Since that is not possible, the span is equal to  $\mathcal{C}(\mathbf{A})$  and  $\dim(\mathcal{C}(\mathbf{A})) = n - k = r = \text{rank}(\mathbf{A})$ , so that  $k = \dim(\mathcal{N}(\mathbf{A})) = n - r$ .

Interpretation: “dimension of column space + dimension of null space = # columns”

Mis-Interpretation: Columns space and null space are orthogonal complement to each other.

They are of different orders in general! Next result gives the correct statement.

Reference:

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

## Probability theory review

A few basic elements to define a probability on a set:

- **Sample space**  $S$  is the set that contains all possible outcomes of a particular experiment.
- An **event** is any collection of possible outcomes of an experiment, that is, any subset of  $S$  (including  $S$  itself).
- Event operations
  1. Union: The union of  $A$  and  $B$ , written  $A \cup B$ , is the set of elements that belong to either  $A$  or  $B$  or both:

$$A \cup B = \{x : x \in A \text{ or } x \in B\}$$

2. Intersection: The intersection of  $A$  and  $B$ , written  $A \cap B$ , is the set of elements that belong to both  $A$  and  $B$ :

$$A \cap B = \{x : x \in A \text{ and } x \in B\}$$

3. Complementation: The complement of  $A$ , written as  $A^c$ , is the set of all elements that are not in  $A$ :

$$A^c = \{x : x \notin A\}.$$

- **Sigma algebra (or Borel field):** A collection of subsets of  $S$  is called a sigma algebra (or Borel field), denoted by  $\mathcal{B}$ , if it satisfies the following three properties:
  1.  $\emptyset \in \mathcal{B}$  (the empty set is an element of  $\mathcal{B}$ )
  2. If  $A \in \mathcal{B}$ , then  $A^c \in \mathcal{B}$  ( $\mathcal{B}$  is closed under complementation).
  3. If  $A_1, A_2, \dots \in \mathcal{B}$ , then  $\cup_{i=1}^{\infty} A_i \in \mathcal{B}$  ( $\mathcal{B}$  is closed under countable unions).
- **Axioms of probability:** Given a sample space  $S$  and an associated sigma algebra  $\mathcal{B}$ , a *probability function* is a function  $\Pr()$  with domain  $\mathcal{B}$  that satisfies
  1.  $\Pr(A) \geq 0$  for all  $A \in \mathcal{B}$
  2.  $\Pr(S) = 1$ .
  3. If  $A_1, A_2, \dots \in \mathcal{B}$  are pairwise disjoint, then  $\Pr(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \Pr(A_i)$ .

### Properties:

If  $\Pr()$  is a *probability function* and  $A$  and  $B$  are any sets in  $\mathcal{B}$ , then

- $\Pr(\emptyset) = 0$ , where  $\emptyset$  is the empty set  
*Proof:*  $1 = \Pr(S) = \Pr(S \cup \emptyset)$
- $\Pr(A) \leq 1$   
*Proof:* see below and remember  $\Pr(A^c) \geq 0$
- $\Pr(A^c) = 1 - \Pr(A)$   
*Proof:*  $1 = \Pr(S) = \Pr(A \cup A^c) = \Pr(A) + \Pr(A^c)$
- $\Pr(B \cap A^c) = \Pr(B) - \Pr(A \cap B)$   
*Proof:*  $B = \{B \cap A\} \cup \{B \cap A^c\}$
- $\Pr(A \cup B) = \Pr(A) + \Pr(B) - \Pr(A \cap B)$   
*Proof:*  $A \cup B = A \cup \{B \cap A^c\}$  and use the above property.
- $\Pr(A \cup B) = \Pr(A) + \Pr(B \cap A^c) = \Pr(A) + \Pr(B) - \Pr(A \cap B)$
- If  $A \subset B$ , then  $\Pr(A) \leq \Pr(B)$ .  
*Proof:* If  $A \subset B$ , then  $A \cap B = A$  and use  $\Pr(B \cap A^c) = \Pr(B) - \Pr(A \cap B)$ .

### Conditional probability

*Definition:* If  $A$  and  $B$  are events in  $S$ , and  $\Pr(B) > 0$ , then the conditional probability of  $A$  given  $B$ , written  $\Pr(A|B)$ , is

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)}$$

Note that what happens in the conditional probability calculation is that  $B$  becomes the sample space:  $\Pr(B|B) = 1$ , in other words,  $\Pr(A|B)$  is the probability measure of the event  $A$  after observing the occurrence of event  $B$ .

*Definition:* Two events  $A$  and  $B$  are statistically independent if  $\Pr(A \cap B) = \Pr(A) \Pr(B)$ . When  $A$  and  $B$  are independent events, then  $\Pr(A|B) = \Pr(A)$  and the following pairs are also independent

- $A$  and  $B^c$   
*proof:*

$$\begin{aligned}\Pr(A \cap B^c) &= \Pr(A) - \Pr(A \cap B) \\ &= \Pr(A) - \Pr(A) \Pr(B) \\ &= \Pr(A)(1 - \Pr(B)) \\ &= \Pr(A) \Pr(B^c)\end{aligned}$$

- $A^c$  and  $B$
- $A^c$  and  $B^c$

## Random variables

*Definition:* A random variable is a function from a sample space  $S$  into the real numbers.

Experiment	Random variable
Toss two dice	$X = \text{sum of the numbers}$
Toss a coin 25 times	$X = \text{number of heads in 25 tosses}$
Apply different amounts of fertilizer to corn plants	$X = \text{yield/acre}$

Suppose we have a sample space

$$S = \{s_1, \dots, s_n\}$$

with a probability function  $\Pr$  and we define a random variable  $X$  with range  $\mathcal{X} = \{x_1, \dots, x_m\}$ . We can define a probability function  $\Pr_X$  on  $\mathcal{X}$  in the following way. We will observe  $X = x_i$  if and only if the outcome of the random experiment is an  $s_j \in S$  such that  $X(s_j) = x_i$ . Thus,

$$\Pr_X(X = x_i) = \Pr(\{s_j \in S : X(s_j) = x_i\}).$$

We will simply write  $\Pr(X = x_i)$  rather than  $\Pr_X(X = x_i)$ .

*A note on notation:* Random variables are often denoted with uppercase letters and the realized values of the variables (or its range) are denoted by corresponding lowercase letters.

## Distribution functions

*Definition:* The cumulative distribution function or cdf of a random variable (r.v.)  $X$ , denoted by  $F_X(x)$  is defined by

$$F_X(x) = \Pr(X \leq x), \text{ for all } x.$$

The function  $F(x)$  is a cdf if and only if the following three conditions hold:

1.  $\lim_{x \rightarrow \infty} F(x) = 1$ .
2.  $F(x)$  is a nondecreasing function of  $x$ .
3.  $F(x)$  is right-continuous; that is, for every number  $x_0$ ,  $\lim_{x \downarrow x_0} F(x) = F(x_0)$ .

*Definition:* A random variable  $X$  is continuous if  $F(x)$  is a continuous function of  $x$ . A random variable  $X$  is discrete if  $F(x)$  is a step function of  $x$ .

The following two statements are equivalent:

1. The random variables  $X$  and  $Y$  are identically distributed.
2.  $F_X(x) = F_Y(x)$  for every  $x$ .

## Density and mass functions

*Definition:* The probability mass function (pmf) of a discrete random variable  $X$  is given by

$$f_X(x) = \Pr(X = x) \text{ for all } x.$$

*Example (Geometric probabilities)* For the geometric distribution, we have the pmf

$$f_X(x) = \Pr(X = x) = \begin{cases} p(1-p)^{x-1} & \text{for } x = 1, 2, \dots \\ 0 & \text{otherwise.} \end{cases}$$

*Definition:* The probability density function or pdf,  $f_X(x)$ , of a continuous random variable  $X$  is the function that satisfies

$$F_X(x) = \int_{-\infty}^x f_X(t)dt \quad \text{for all } x.$$

*A note on notation:* The expression “ $X$  has a distribution given by  $F_X(x)$ ” is abbreviated symbolically by “ $X \sim F_X(x)$ ”, where we read the symbol “ $\sim$ ” as “is distributed as”.

*Example (Logistic distribution)* For the logistic distribution, we have

$$F_X(x) = \frac{1}{1 + e^{-x}}$$

and, hence,

$$f_X(x) = \frac{d}{dx}F_X(x) = \frac{e^{-x}}{(1 + e^{-x})^2}.$$

A function  $f_X(x)$  is a pdf (or pmf) of a random variable  $X$  if and only if

1.  $f_X(x) \geq 0$  for all  $x$
2.  $\sum_x f_X(x) = 1$  (pmf) or  $\int_{-\infty}^{\infty} f_X(x)dx = 1$  (pdf).

## Expectations

The expected value, or expectation, of a random variable is merely its average value, where we speak of “average” value as one that is weighted according to the probability distribution.

*Definition:* The expected value or mean of a random variable  $g(X)$ , denoted by  $\mathbf{E}(g(X))$ , is

$$\mathbf{E}(g(X)) = \begin{cases} \int_{-\infty}^{\infty} g(x)f_X(x)dx & \text{if } X \text{ is continuous} \\ \sum_{x \in \mathcal{X}} g(x)f_X(x) = \sum_{x \in \mathcal{X}} g(x)\Pr(X = x) & \text{if } X \text{ is discrete,} \end{cases}$$

## Exponential mean

Suppose  $X \sim \text{Exp}(\lambda)$  distribution, that is, it has pdf given by

$$f_X(x) = \frac{1}{\lambda}e^{-x/\lambda}, \quad 0 \leq x < \infty, \quad \lambda > 0$$



Then  $\mathbf{E}(X)$  is:

$$\begin{aligned}\mathbf{E}(X) &= \int_0^\infty \frac{1}{\lambda} x e^{-x/\lambda} dx \\ &= -x e^{-x/\lambda} \Big|_0^\infty + \int_0^\infty e^{-x/\lambda} dx \\ &= \int_0^\infty e^{-x/\lambda} dx = \lambda\end{aligned}$$

### Binomial mean

IF  $X$  has binomial distribution, i.e.  $X \sim \text{binomial}(n, p)$ , its pmf is given by

$$\Pr(X = x) = \binom{n}{x} p^x (1-p)^{n-x}, \quad x = 0, 1, \dots, n,$$

where  $n$  is a positive integer,  $0 \leq p \leq 1$ , and for every fixed pair  $n$  and  $p$  the pmf sums to 1. The expected value of a binomial random variable is then given by

$$\mathbf{E}(X) = \sum_{x=0}^n x \binom{n}{x} p^x (1-p)^{n-x}$$

Now, use the identity  $x \binom{n}{x} = n \binom{n-1}{x-1}$  to derive the Expected value.

$$\begin{aligned}\mathbf{E}(X) &= \sum_{x=1}^n x \binom{n}{x} p^x (1-p)^{n-x} \\ &= \sum_{x=1}^n n \binom{n-1}{x-1} p^x (1-p)^{n-x} \\ &= \sum_{y=0}^{n-1} n \binom{n-1}{y} p^{y+1} (1-p)^{n-(y+1)} \\ &= np \sum_{y=0}^{n-1} \binom{n-1}{y} p^y (1-p)^{n-1-y} \\ &= np,\end{aligned}$$

since the last summation must be 1, being the sum over all possible values of a  $\text{binomial}(n-1, p)$  pmf.

properties:

Let  $X$  be a random variable and let  $a, b$  and  $c$  be constants. Then for any functions  $g_1(x)$  and  $g_2(x)$  whose expectations exist,

$$1. \quad \mathbf{E}(a \cdot g_1(X) + b \cdot g_2(X) + c) = a\mathbf{E}(g_1(X)) + b\mathbf{E}(g_2(X)) + c.$$

2. If  $g_1(x) \geq 0$  for all  $x$ , then  $\mathbf{E}(g_1(X)) \geq 0$ .
3. If  $g_1(x) \geq g_2(x)$  for all  $x$ , then  $\mathbf{E}(g_1(X)) \geq \mathbf{E}(g_2(X))$ .
4. If  $a \leq g_1(x) \leq b$  for all  $x$ , then  $a \leq \mathbf{E}(g_1(X)) \leq b$ .

## Moments

The various moments of a distribution are an important class of expectations.

*Definition:* For each integer  $n$ , the  $n^{th}$  moment of  $X$  (or  $F_X(x)$ ),  $\mu'_n$ , is

$$\mu'_n = \mathbf{E}(X^n).$$

The  $n^{th}$  central moment of  $X$ ,  $\mu_n$ , is

$$\mu_n = \mathbf{E}((X - \mu)^n),$$

where  $\mu = \mu'_1 = \mathbf{E}(X)$ .

## Variance

*Definition:* The variance of a random variable  $X$  is its second central moment,  $\mathbf{Var}(X) = \mathbf{E}((X - EX)^2)$ . The positive square root of  $\mathbf{Var}(X)$  is the standard deviation of  $X$ .

## Exponential variance

Let  $X$  have the exponential( $\lambda$ ) distribution,  $X \sim \text{Exp}(\lambda)$ . Then the variance of  $X$  is

$$\begin{aligned} \mathbf{Var}(X) &= \mathbf{E}((X - EX)^2) = \mathbf{E}((X - \lambda)^2) \\ &= \int_0^\infty (x - \lambda)^2 \frac{1}{\lambda} e^{-x/\lambda} dx \\ &= \int_0^\infty (x^2 - 2x\lambda + \lambda^2) \frac{1}{\lambda} e^{-x/\lambda} dx \\ &= \lambda^2. \end{aligned}$$

## properties

1.  $\mathbf{Var}(aX + b) = a^2 \mathbf{Var}(X)$ .

*proof:*

$$\begin{aligned} \mathbf{Var}(aX + b) &= \mathbf{E}(((aX + b) - \mathbf{E}(aX + b))^2) \\ &= \mathbf{E}((aX - aEX)^2) \\ &= a^2 \mathbf{E}((X - EX)^2) \\ &= a^2 \mathbf{Var}(X) \end{aligned}$$

$$2. \text{Var}(X) = \mathbf{E}(X^2) - (\mathbf{E}(X))^2.$$

*proof:*

$$\begin{aligned} \text{Var}(X) &= \mathbf{E}(X - EX)^2 \\ &= \mathbf{E}(X^2 - 2X\mathbf{E}(X) + (\mathbf{E}(X))^2) \\ &= \mathbf{E}(X^2) - 2\mathbf{E}(X)\mathbf{E}(X) + (\mathbf{E}(X))^2 \\ &= \mathbf{E}(X^2) - (\mathbf{E}(X))^2 \end{aligned}$$

### Moment generating function

*Definition:* Let  $X$  be a random variable with cdf  $F_X$ . The moment generating function or mgf of  $X$  (or  $F_X$ ), denoted by  $M_X(t)$ , is

$$M_X(t) = \mathbf{E}(e^{tX}),$$

provided that the expectation exists for  $t$  in some neighborhood of 0. That is, there exists an  $h > 0$  such that for all  $t$  in  $-h < t < h$ ,  $\mathbf{E}(e^{tX})$  exists. If the expectation does not exist in a neighborhood of 0, we say that the moment generating function does not exist.

*Property:* If  $X$  has mgf  $M_X(t)$ , then

$$\mathbf{E}(X^n) = M_X^{(n)}(0),$$

where we define

$$M_X^{(n)}(0) = \left. \frac{d^n}{dt^n} M_X(t) \right|_{t=0}.$$

## 7 Lecture 7: Feb 6

Last time

- R basics

Today

- Simple Linear Regression (JF Chapter 5)

### Simple linear regression

Figure 7.1 shows Davis's data on the measured and reported weight in kilograms of 101 women who were engaged in regular exercise.

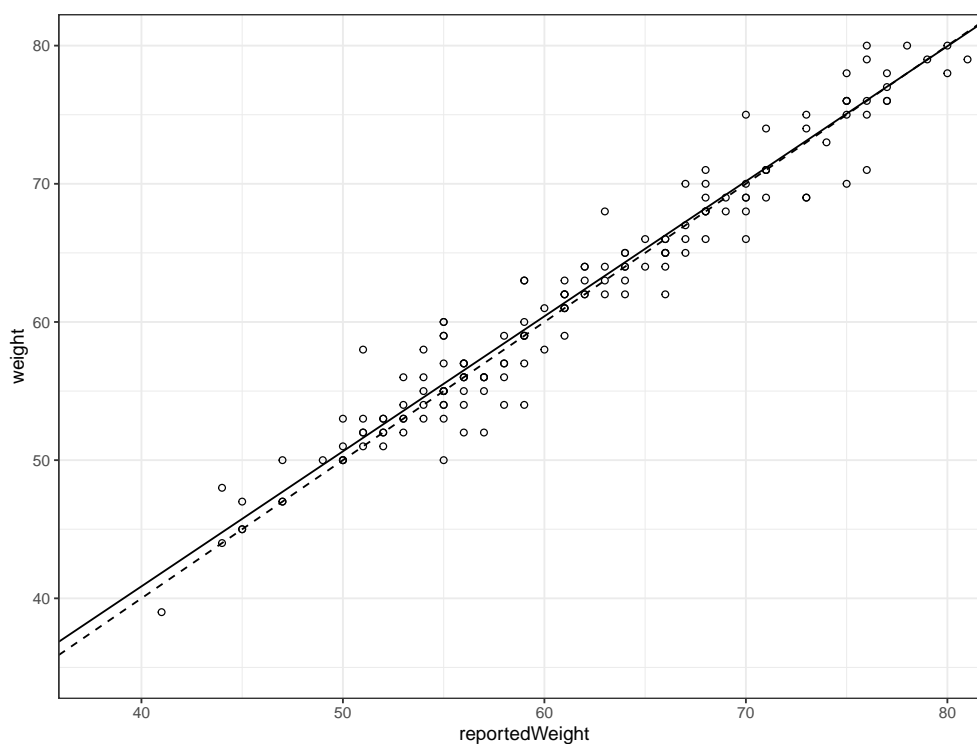


Figure 7.1: Scatterplot of Davis's data on the measured and reported weight of 101 women. The dashed line gives  $y = x$ .

It's reasonable to assume that the relationship between measured and reported weight appears to be linear. Denote:

- measured weight by  $y_i$ : **response variable** or **dependent variable**
- reported weight by  $x_i$ : **predictor variable** or **independent variable**
- intercept:  $\beta_0$

- slope:  $\beta_1$
- residual/error term  $\epsilon_i$ .

Then the simple linear regression model writes:

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

For given  $(\hat{\beta}_0, \hat{\beta}_1)$  values, the *fitted value* or *predicted value* for observation  $i$  is:

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

Therefore, the residual is

$$\hat{\epsilon}_i = y_i - \hat{y}_i$$

### Fitting a linear model

Choose the “best” values for  $\beta_0, \beta_1$  such that

$$SS[E] = \sum_1^n \left( y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i) \right)^2 = \sum_1^n (y_i - \hat{y}_i)^2 = \sum_1^n \epsilon_i^2$$

is minimized. These are **least squares** (LS) estimates:

$$\begin{aligned}\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}.\end{aligned}$$

*Definition:* The line satisfying the equation

$$y = \hat{\beta}_0 + \hat{\beta}_1 x$$

is called the linear regression of  $y$  on  $x$  which is also called the least squares line.

For Davis’s data, we have

$$\begin{aligned}n &= 101 \\ \bar{y} &= \frac{5780}{101} = 57.228 \\ \bar{x} &= \frac{5731}{101} = 56.743 \\ \sum (x_i - \bar{x})(y_i - \bar{y}) &= 4435.9 \\ \sum (x_i - \bar{x})^2 &= 4539.3,\end{aligned}$$

so that

$$\begin{aligned}\hat{\beta}_1 &= \frac{4435.9}{4539.3} = 0.97722 \\ \hat{\beta}_0 &= 57.228 - 0.97722 \times 56.743 = 1.7776\end{aligned}$$

## Least squares estimates

The simple linear regression (SLR) model writes:

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

The least squares estimates minimizes the sum of squared error (SSE) which is

$$SS[E] = \sum_1^n \left( y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i) \right)^2 = \sum_1^n (y_i - \hat{y}_i)^2 = \sum_1^n \hat{\epsilon}_i^2.$$

The **least squares** (LS) estimates (in vector form):

$$\hat{\beta}_{ls} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} = \begin{pmatrix} \bar{y} - \hat{\beta}_1 \bar{x} \\ \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \end{pmatrix}.$$

*Definition:* The line satisfying the equation

$$y = \hat{\beta}_0 + \hat{\beta}_1 x$$

is called the linear regression of  $y$  on  $x$  which is also called the least squares line.

## SLR Model in Matrix Form

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 x_1 \\ \beta_0 + \beta_1 x_2 \\ \vdots \\ \beta_0 + \beta_1 x_n \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

## Jargons

- $\mathbf{X}$  is called the *design matrix*
- $\boldsymbol{\beta}$  is the vector of parameters
- $\boldsymbol{\epsilon}$  is the error vector
- $\mathbf{Y}$  is the response vector.

The Design Matrix

$$\mathbf{X}_{n \times 2} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

Vector of Parameters

$$\boldsymbol{\beta}_{2 \times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

Vector of Error terms

$$\boldsymbol{\epsilon}_{n \times 1} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Vector of Responses

$$\mathbf{Y}_{n \times 1} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Gramian Matrix

$$\mathbf{X}^T \mathbf{X} = \begin{bmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{bmatrix}$$

Therefore, we have

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

Assume the Gramian matrix has full rank (which actually should be the case, why?), we want to show that

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

The inverse of the Gramian matrix is

$$(\mathbf{X}^T \mathbf{X})^{-1} = \frac{1}{n \sum_i (x_i - \bar{x})^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix}$$

Now we have

$$\begin{aligned}
\hat{\beta}_{ls} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \\
&= \frac{1}{n \sum_i (x_i - \bar{x})^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix} \begin{bmatrix} \mathbf{1}_n^T \\ \mathbf{x}^T \end{bmatrix} \mathbf{y} \\
&= \frac{1}{n \sum_i (x_i - \bar{x})^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix} \begin{bmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{bmatrix} \\
&= \frac{1}{n \sum_i (x_i - \bar{x})^2} \begin{bmatrix} (\sum_i x_i^2)(\sum_i y_i) - (\sum_i x_i)(\sum_i x_i y_i) \\ n \sum_i x_i y_i - (\sum_i x_i)(\sum_i y_i) \end{bmatrix} \\
&= \begin{bmatrix} \bar{y} - \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \bar{x} \\ \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \end{bmatrix}
\end{aligned}$$



## 9 Lecture 9: Feb 8

Last time

- Introduction of simple linear regression

Today

- Simple correlation

*From last lecture:* Assume the Gramian matrix has full rank (which actually should be the case, why?)

$$\mathbf{X}^T \mathbf{X} = \begin{bmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{bmatrix}$$

*Proof:* By Cauchy-Schwarz inequality, we have

$$n \sum_i x_i^2 \geq (\sum_i x_i)^2$$

where the equality holds only if all  $x_i$  are equal.

Some properties:

- (a)  $\sum x_i \hat{\epsilon}_i = 0$ .
- (b)  $\sum \hat{y}_i \hat{\epsilon}_i = 0$  (HW1).

*Proof:* For (a), we look at

$$\begin{aligned} & \mathbf{X}^T \hat{\epsilon} \\ &= \mathbf{X}^T (\mathbf{Y} - \mathbf{X} \hat{\beta}) \\ &= \mathbf{X}^T [\mathbf{Y} - \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}] \\ &= \mathbf{X}^T \mathbf{Y} - \mathbf{X}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \\ &= \mathbf{X}^T \mathbf{Y} - \mathbf{X}^T \mathbf{Y} \\ &= \mathbf{0} \end{aligned}$$

### Other quantities in Matrix Form

Fitted values

$$\hat{\mathbf{Y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 + \hat{\beta}_1 x_1 \\ \hat{\beta}_0 + \hat{\beta}_1 x_2 \\ \vdots \\ \hat{\beta}_0 + \hat{\beta}_1 x_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \mathbf{X} \hat{\beta}$$

Hat matrix

$$\begin{aligned}\hat{\mathbf{Y}} &= \mathbf{X}\hat{\boldsymbol{\beta}} \\ \hat{\mathbf{Y}} &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ \hat{\mathbf{Y}} &= \mathbf{H}\mathbf{Y}\end{aligned}$$

where  $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$  is called “hat matrix” because it turns  $\mathbf{Y}$  into  $\hat{\mathbf{Y}}$ .

## Simple correlation

Having calculated the least squares line, it is of interest to determine how closely the line fits the scatter of points. There are many ways of answering it. The standard deviation of the residuals,  $S_E$ , often called the *standard error of the regression* or the *residue standard error*, provides one sort of answer. Because of estimation considerations, the variance of the residuals is defined using *degrees of freedom*  $n - 2$ :

$$S_\epsilon^2 = \frac{\sum \hat{\epsilon}_i^2}{n - 2}.$$

The residual standard error is,

$$S_\epsilon = \sqrt{\frac{\sum \hat{\epsilon}_i^2}{n - 2}}$$

For the Davis’s data, the sum of squared residuals is  $\sum \hat{\epsilon}_i^2 = 418.87$ , and thus the standard error of the regression is

$$S_\epsilon = \sqrt{\frac{418.87}{101 - 2}} = 2.0569\text{kg}.$$

On average, using the least-squares regression line to predict measured weight from reported weight results in an error of about 2 kg.

*Sum of squares:*

- Total sum of squares (TSS) for Y:  $\text{TSS} = \sum (y_i - \bar{y})^2$
- Residual sum of squares (RSS):  $\text{RSS} = \sum (y_i - \hat{y}_i)^2$
- regression sum of squares (RegSS):  $\text{RegSS} = \text{TSS} - \text{RSS} = \sum (\hat{y}_i - \bar{y})^2$
- $\text{RegSS} + \text{RSS} = \text{TSS}$

## Sample correlation coefficient

*Definition:* The sample correlation coefficient  $r_{xy}$  of the paired data  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  is defined by

$$r_{xy} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y}) / (n - 1)}{\sqrt{\sum (x_i - \bar{x})^2 / (n - 1) \times \sum (y_i - \bar{y})^2 / (n - 1)}} = \frac{s_{xy}}{s_x s_y}$$

$s_{xy}$  is called the sample covariance of  $x$  and  $y$ :

$$s_{xy} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n - 1}$$

$s_x = \sqrt{\sum (x_i - \bar{x})^2 / (n - 1)}$  and  $s_y = \sqrt{\sum (y_i - \bar{y})^2 / (n - 1)}$  are, respectively, the sample standard deviations of  $X$  and  $Y$ .

Some properties of  $r_{xy}$ :

- $r_{xy}$  is a measure of the linear association between  $x$  and  $y$  in a dataset.
- correlation coefficients are always between  $-1$  and  $1$ :

$$-1 \leq r_{xy} \leq 1$$

- The closer  $r_{xy}$  is to  $1$ , the stronger the positive linear association between  $x$  and  $y$
- The closer  $r_{xy}$  is to  $-1$ , the stronger the negative linear association between  $x$  and  $y$
- The bigger  $|r_{xy}|$ , the stronger the linear association
- If  $|r_{xy}| = 1$ , then  $x$  and  $y$  are said to be perfectly correlated.
- $\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} = r_{xy} \frac{s_y}{s_x}$

## 11 Lecture 11: Feb 13

### Last time

- Introduction of simple linear regression

### Today

- HW2 posted
- The statistical model of the SLR (JF chapter 6)
- Properties of the Least-Squares estimator
- Inference of SLR model

### R-square

The ratio of RegSS to TSS is called the *coefficient of determination*, or sometimes, simply “r-square”. it represents the proportion of variation observed in the response variable  $y$  which can be “explained” by its linear association with  $x$ .

- In simple linear regression, “r-square” is in fact equal to  $r_{xy}^2$ . (But this isn’t the case in multiple regression.)
- It is also equal to the squared correlation between  $y_i$  and  $\hat{y}_i$ . (This is the case in multiple regression.)

For Davis’s regression of measured on reported weight:

$$\text{TSS} = 4753.8$$

$$\text{RSS} = 418.87$$

$$\text{RegSS} = 4334.9$$

Thus,

$$r^2 = \frac{4334.9}{4753.8} = 1 - \frac{418.87}{4753.8} = 0.9119$$

## The statistical model of Simple Linear Regression

Standard statistical inference in simple regression is based on a *statistical model* that describes the population or process that is sampled:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where the coefficients  $\beta_0$  and  $\beta_1$  are the *population regression parameters*. The data are randomly sampled from some population of interest.

- $y_i$  is the value of the response variable

- $x_i$  is the explanatory variable
- $\epsilon_i$  represents the aggregated omitted causes of  $y$  (i.e., the causes of  $y$  beyond the explanatory variable), other explanatory variables that could have been included in the regression model, measurement error in  $y$ , and whatever component of  $y$  is inherently random.

## Key assumptions of SLR

The key assumptions of the SLR model concern the behavior of the errors, equivalently, the distribution of  $y$  conditional on  $x$ :

- *Linearity.* The expectation of the error given the value of  $x$  is 0:  $\mathbf{E}(\epsilon) \equiv \mathbf{E}(\epsilon|x_i) = 0$ . And equivalently, the expected value of the response variable is a linear function of the explanatory variable:  $\mu_i \equiv \mathbf{E}(y_i) \equiv \mathbf{E}(y_i|x_i) = \mathbf{E}(\beta_0 + \beta_1 x_i + \epsilon_i|x_i) = \beta_0 + \beta_1 x_i$ .
- *Constant variance.* The variance of the errors is the same regardless of the value of  $x$ :  $\mathbf{Var}(\epsilon|x_i) = \sigma_\epsilon^2$ . The constant error variance implies constant conditional variance of  $y$  on given  $x$ :  $\mathbf{Var}(y|x_i) = \mathbf{E}((y_i - \mu_i)^2) = \mathbf{E}((y_i - \beta_0 - \beta_1 x_i)^2) = \mathbf{E}(\epsilon_i^2) = \sigma_\epsilon^2$ . (Question: why the last equal sign?)
- *Normality.* The errors are independent identically distributed with Normal distribution with mean 0 and variance  $\sigma_\epsilon^2$ . Write as  $\epsilon_i \stackrel{iid}{\sim} N(0, \sigma_\epsilon^2)$ . Equivalently, the conditional distribution of the response variable is normal:  $y_i \stackrel{iid}{\sim} N(\beta_0 + \beta_1 x_i, \sigma_\epsilon^2)$ .
- *Independence.* The observations are sampled independently.
- *Fixed  $X$ , or  $X$  measured without error and independent of the error.*
  - For experimental research where  $X$  values are under direct control of the researcher (i.e.  $X$ 's are fixed). If the experiment were replicated, then the values of  $X$  would remain the same.
  - For research where  $X$  values are sampled, we assume the explanatory variable is measured without error and the explanatory variable and the error are independent in the population from which the sample is drawn.
- *$X$  is not invariant.*  $X$ 's can not be all the same.

Figure 11.1 shows the assumptions of linearity, constant variance, and normality in SLR model.



Figure 11.1: The assumptions of linearity, constant variance, and normality in simple regression. The graph shows the conditional population distributions  $\Pr(Y|x)$  of  $Y$  for several values of the explanatory variable  $X$ , labeled as  $x_1, x_2, \dots, x_5$ . The conditional means of  $Y$  given  $x$  are denoted  $\mu_1, \dots, \mu_5$ .

## Properties of the Least-Squares estimator

Under the strong assumptions of the simple regression model, the sample least squares coefficients  $\hat{\beta}_{ls}$  have several desirable properties as estimators of the population regression coefficients  $\beta_0$  and  $\beta_1$ :

- The least-squares intercept and slope are *linear estimators*, in the sense that they are linear functions of the observations  $y_i$ .

*Proof:*

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

method (b)  $\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{\sum (x_i - \bar{x})y_i}{\sum (x_i - \bar{x})^2} - \frac{\sum (x_i - \bar{x})\bar{y}}{\sum (x_i - \bar{x})^2} = \sum \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2} y_i = \sum k_i y_i$  where

$$k_i = \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2}$$

and  $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$

- The sample least-squares coefficients are *unbiased estimators* of the population regression coefficients:

$$\mathbf{E}(\hat{\beta}_0) = \beta_0$$

$$\mathbf{E}(\hat{\beta}_1) = \beta_1$$

*Proof:*

method (a)  $\mathbf{E}(\hat{\beta}) = \mathbf{E}((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}) = \mathbf{E}((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X} \beta) = \beta$ . (note:  $\mathbf{E}(Y) = \mathbf{E}(\mathbf{X}\beta + \epsilon) = \mathbf{E}(\mathbf{X}\beta) + \mathbf{E}(\epsilon) = \mathbf{X}\beta$ )

method (b) recall that  $\hat{\beta}_1 = \sum k_i y_i$  where  $k_i = \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2}$ . First, we want to show

1.  $\sum k_i = 0$
2.  $\sum k_i x_i = 1$

They are actually quite easy:  $\sum k_i = \sum_i \frac{(x_i - \bar{x})}{\sum_j (x_j - \bar{x})^2} = \frac{(\sum_i x_i) - n\bar{x}}{\sum_j (x_j - \bar{x})^2} = 0$ , and  $\sum k_i x_i = \sum_i \frac{(x_i - \bar{x})x_i}{\sum_j (x_j - \bar{x})^2} = \frac{(\sum_i x_i^2) - \bar{x}(\sum_i x_i)}{\sum_j (x_j - \bar{x})^2} = \frac{(\sum_i x_i^2) - n\bar{x}^2}{\sum_j (x_j - \bar{x})^2} = 1$ .

Now  $\mathbf{E}(\hat{\beta}_1) = \mathbf{E}(\sum k_i y_i) = \sum [k_i \mathbf{E}(y_i)] = \sum [k_i(\beta_0 + \beta_1 x_i)] = \beta_0 \sum k_i + \beta_1 \sum (k_i x_i) = \beta_1$ , and  $\mathbf{E}(\hat{\beta}_0) = \mathbf{E}(\bar{y} - \hat{\beta}_1 \bar{x}) = \mathbf{E}(\bar{y}) - \bar{x} \mathbf{E}(\hat{\beta}_1) = \mathbf{E}(\frac{1}{n} \sum y_i) - \bar{x} \beta_1 = \frac{1}{n} [\sum \mathbf{E}(y_i)] - \bar{x} \beta_1 = \frac{1}{n} \sum [\beta_0 + x_i \beta_1] - \bar{x} \beta_1 = \beta_0$

- Both  $\hat{\beta}_0$  and  $\hat{\beta}_1$  have simple sampling variances:

$$\text{Var}(\hat{\beta}_0) = \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}$$

*Proof:*

$\text{Var}(\hat{\beta}_1) = \text{Var}(\sum k_i y_i) = \sum k_i^2 \text{Var}(y_i) = \sigma_\epsilon^2 \sum k_i^2 = \sigma_\epsilon^2 \frac{\sum_i (x_i - \bar{x})^2}{[\sum_j (x_j - \bar{x})^2]^2} = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}$ , and

$\text{Var}(\hat{\beta}_0) = \text{Var}(\bar{y} - \hat{\beta}_1 \bar{x}) = \text{Var}(\bar{y}) + (\bar{x})^2 \text{Var}(\hat{\beta}_1) - 2\bar{x} \text{Cov}(\bar{Y}, \hat{\beta}_1)$ .

Now,

$$\text{Var}(\bar{y}) = \text{Var}\left(\frac{1}{n} \sum_{i=1}^n y_i\right) = \frac{1}{n^2} \sum_{i=1}^n \text{Var}(y_i) = \frac{\sigma^2}{n},$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2},$$

and

$$\begin{aligned} \text{Cov}(\bar{Y}, \hat{\beta}_1) &= \text{Cov}\left\{\frac{1}{n} \sum_{i=1}^n Y_i, \frac{\sum_{j=1}^n (x_j - \bar{x}) Y_j}{\sum_{i=1}^n (x_i - \bar{x})^2}\right\} \\ &= \frac{1}{n} \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \text{Cov}\left\{\sum_{i=1}^n Y_i, \sum_{j=1}^n (x_j - \bar{x}) Y_j\right\} \\ &= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_j - \bar{x}) \sum_{j=1}^n \text{Cov}(Y_i, Y_j) \\ &= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_j - \bar{x}) \sigma^2 \\ &= 0. \end{aligned}$$

Finally,

$$\begin{aligned}\text{Var}(\hat{\beta}_0) &= \frac{\sigma^2}{n} + \frac{\sigma^2 \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sigma^2}{n \sum_{i=1}^n (x_i - \bar{x})^2} \left\{ \sum_{i=1}^n (x_i - \bar{x})^2 + n \bar{x}^2 \right\} \\ &= \frac{\sigma^2 \sum_{i=1}^n x_i^2}{n \sum_{i=1}^n (x_i - \bar{x})^2}.\end{aligned}$$

- Rewrite the formula for  $\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{(n-1)S_X^2}$ , we see that the sampling variance of the slope estimate will be small when
  - The error variance  $\sigma_\epsilon^2$  is small
  - The sample size  $n$  is large
  - The explanatory-variable values are spread out (i.e. have a large variance,  $S_X^2$ )

- (Gauss-Markov theorem) Under the assumptions of linearity, constant variance, and independence, the least-squares estimators are BLUE (Best Linear Unbiased Estimator), that is they have the smallest sampling variance and are unbiased. (show this)

*Proof:*

Let  $\tilde{\beta}_1$  be another linear unbiased estimator such that  $\tilde{\beta}_1 = \sum c_i y_i$ . For  $\tilde{\beta}_1$  is still unbiased as above,  $\mathbf{E}(\tilde{\beta}_1) = \beta_0 \sum c_i + \beta_1 \sum c_i x_i = \beta_1$  for all  $\beta_1$ , we have  $\sum c_i = 0$  and  $\sum c_i x_i = 1$ .

$$\mathbf{Var}(\tilde{\beta}_1) = \sigma_\epsilon^2 \sum c_i^2$$

Let  $c_i = k_i + d_i$ , then

$$\begin{aligned}\mathbf{Var}(\tilde{\beta}_1) &= \sigma_\epsilon^2 \sum (k_i + d_i)^2 \\ &= \sigma_\epsilon^2 \left[ \sum k_i^2 + \sum d_i^2 + 2 \sum k_i d_i \right] \\ &= \mathbf{Var}(\hat{\beta}_1) + \sigma_\epsilon^2 \sum d_i^2 + 2\sigma_\epsilon^2 \sum k_i d_i\end{aligned}$$

Now we show the last term is 0 to finish the proof.

$$\begin{aligned}\sum k_i d_i &= \sum k_i (c_i - k_i) = \sum c_i k_i - \sum k_i^2 \\ &= \sum_i \left[ c_i \frac{x_i - \bar{x}}{\sum_j (x_j - \bar{x})^2} \right] - \frac{1}{\sum_i (x_i - \bar{x})^2} \\ &= 0\end{aligned}$$

- Under the full suite of assumptions, the least-squares coefficients  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are the maximum-likelihood estimators of  $\beta_0$  and  $\beta_1$ . (show this)



*Proof:*

The log likelihood under the full suite of assumptions is  $\ell = -\log \left[ (2\pi)^{\frac{n}{2}} \sigma_\epsilon^n \right] - \frac{1}{2\sigma_\epsilon^2} (\mathbf{Y} - \mathbf{X}\beta)^T (\mathbf{Y} - \mathbf{X}\beta)$ . Maximizing the likelihood is equivalent as minimizing  $(\mathbf{Y} - \mathbf{X}\beta)^T (\mathbf{Y} - \mathbf{X}\beta) = \epsilon^T \epsilon$  which is the SSE.

- Under the assumption of normality, the least-squares coefficients are themselves normally distributed. Summing up,

$$\hat{\beta}_0 \sim N\left(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}\right)$$

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}\right)$$

## 12 Lecture 12 Feb 15

### Last time

- Properties of the Least-Squares estimator

### Today

- HW1 due Feb 17
- Inference of SLR model
- Multiple linear regression

### Properties of the Least-Squares estimator

Under the strong assumptions of the simple regression model, the sample least squares coefficients  $\hat{\beta}_{ls}$  have several desirable properties as estimators of the population regression coefficients  $\beta_0$  and  $\beta_1$ :

- The least-squares intercept and slope are *linear estimators*, in the sense that they are linear functions of the observations  $y_i$ .

*Proof:*

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

method (b)  $\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{\sum (x_i - \bar{x}) y_i}{\sum (x_i - \bar{x})^2} - \frac{\sum (x_i - \bar{x}) \bar{y}}{\sum (x_i - \bar{x})^2} = \sum \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2} y_i = \sum k_i y_i$  where

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and  $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$

- The sample least-squares coefficients are *unbiased estimators* of the population regression coefficients:

$$\mathbf{E}(\hat{\beta}_0) = \beta_0$$

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*Proof:*

method (a)  $\mathbf{E}(\hat{\beta}) = \mathbf{E}((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}) = \mathbf{E}((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X} \beta) = \beta$ . (note:  $\mathbf{E}(Y) = \mathbf{E}(\mathbf{X}\beta + \epsilon) = \mathbf{E}(\mathbf{X}\beta) + \mathbf{E}(\epsilon) = \mathbf{X}\beta$ )

method (b) recall that  $\hat{\beta}_1 = \sum k_i y_i$  where  $k_i = \frac{(x_i - \bar{x})}{\sum (x_i - \bar{x})^2}$ . First, we want to show

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Now  $\mathbf{E}(\hat{\beta}_1) = \mathbf{E}(\sum k_i y_i) = \sum [k_i \mathbf{E}(y_i)] = \sum [k_i (\beta_0 + \beta_1 x_i)] = \beta_0 \sum k_i + \beta_1 \sum (k_i x_i) =$

$$\beta_1, \text{ and } \mathbf{E}(\hat{\beta}_0) = \mathbf{E}(\bar{y} - \hat{\beta}_1 \bar{x}) = \mathbf{E}(\bar{y}) - \bar{x} \mathbf{E}(\hat{\beta}_1) = \mathbf{E}\left(\frac{1}{n} \sum y_i\right) - \bar{x} \beta_1 = \frac{1}{n} [\sum \mathbf{E}(y_i)] - \bar{x} \beta_1 = \frac{1}{n} \sum [\beta_0 + x_i \beta_1] - \bar{x} \beta_1 = \beta_0$$

- Both  $\hat{\beta}_0$  and  $\hat{\beta}_1$  have simple sampling variances:

$$\text{Var}(\hat{\beta}_0) = \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}$$

*Proof:*

$$\text{Var}(\hat{\beta}_1) = \text{Var}(\sum k_i y_i) = \sum k_i^2 \text{Var}(y_i) = \sigma_\epsilon^2 \sum k_i^2 = \sigma_\epsilon^2 \frac{\sum_i (x_i - \bar{x})^2}{[\sum_j (x_j - \bar{x})^2]^2} = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}, \text{ and}$$

$$\text{Var}(\hat{\beta}_0) = \text{Var}(\bar{y} - \hat{\beta}_1 \bar{x}) = \text{Var}(\bar{y}) + (\bar{x})^2 \text{Var}(\hat{\beta}_1) - 2\bar{x} \text{Cov}(\bar{Y}, \hat{\beta}_1).$$

Now,

$$\text{Var}(\bar{y}) = \text{Var}\left(\frac{1}{n} \sum_{i=1}^n y_i\right) = \frac{1}{n^2} \sum_{i=1}^n \text{Var}(y_i) = \frac{\sigma^2}{n},$$

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2},$$

and

$$\begin{aligned} \text{Cov}(\bar{Y}, \hat{\beta}_1) &= \text{Cov}\left\{\frac{1}{n} \sum_{i=1}^n Y_i, \frac{\sum_{j=1}^n (x_j - \bar{x}) Y_j}{\sum_{i=1}^n (x_i - \bar{x})^2}\right\} \\ &= \frac{1}{n} \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \text{Cov}\left\{\sum_{i=1}^n Y_i, \sum_{j=1}^n (x_j - \bar{x}) Y_j\right\} \\ &= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_j - \bar{x}) \sum_{j=1}^n \text{Cov}(Y_i, Y_j) \\ &= \frac{1}{n \sum_{i=1}^n (x_i - \bar{x})^2} \sum_{i=1}^n (x_j - \bar{x}) \sigma^2 \\ &= 0. \end{aligned}$$

Finally,

$$\begin{aligned} \text{Var}(\hat{\beta}_0) &= \frac{\sigma^2}{n} + \frac{\sigma^2 \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sigma^2}{n \sum_{i=1}^n (x_i - \bar{x})^2} \left\{ \sum_{i=1}^n (x_i - \bar{x})^2 + n \bar{x}^2 \right\} \\ &= \frac{\sigma^2 \sum_{i=1}^n x_i^2}{n \sum_{i=1}^n (x_i - \bar{x})^2}. \end{aligned}$$

- Rewrite the formula for  $\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{(n-1)S_X^2}$ , we see that the sampling variance of the slope estimate will be small when

- The error variance  $\sigma_\epsilon^2$  is small
- The sample size  $n$  is large
- The explanatory-variable values are spread out (i.e. have a large variance,  $S_X^2$ )
- (Gauss-Markov theorem) Under the assumptions of linearity, constant variance, and independence, the least-squares estimators are BLUE (Best Linear Unbiased Estimator), that is they have the smallest sampling variance and are unbiased. (show this)

*Proof:*

Let  $\tilde{\beta}_1$  be another linear unbiased estimator such that  $\tilde{\beta}_1 = \sum c_i y_i$ . For  $\tilde{\beta}_1$  is still unbiased as above,  $\mathbf{E}(\tilde{\beta}_1) = \beta_0 \sum c_i + \beta_1 \sum c_i x_i = \beta_1$  for all  $\beta_1$ , we have  $\sum c_i = 0$  and  $\sum c_i x_i = 1$ .

$$\mathbf{Var}(\tilde{\beta}_1) = \sigma_\epsilon^2 \sum c_i^2$$

Let  $c_i = k_i + d_i$ , then

$$\begin{aligned} \mathbf{Var}(\tilde{\beta}_1) &= \sigma_\epsilon^2 \sum (k_i + d_i)^2 \\ &= \sigma_\epsilon^2 \left[ \sum k_i^2 + \sum d_i^2 + 2 \sum k_i d_i \right] \\ &= \mathbf{Var}(\hat{\beta}_1) + \sigma_\epsilon^2 \sum d_i^2 + 2\sigma_\epsilon^2 \sum k_i d_i \end{aligned}$$

Now we show the last term is 0 to finish the proof.

$$\begin{aligned} \sum k_i d_i &= \sum k_i (c_i - k_i) = \sum c_i k_i - \sum k_i^2 \\ &= \sum_i \left[ c_i \frac{x_i - \bar{x}}{\sum_j (x_j - \bar{x})^2} \right] - \frac{1}{\sum_i (x_i - \bar{x})^2} \\ &= 0 \end{aligned}$$

- Under the full suite of assumptions, the least-squares coefficients  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are the maximum-likelihood estimators of  $\beta_0$  and  $\beta_1$ . (show this)

*Proof:*

The log likelihood under the full suite of assumptions is  $\ell = -\log \left[ (2\pi)^{\frac{n}{2}} \sigma_\epsilon^n \right] - \frac{1}{2\sigma_\epsilon^2} (\mathbf{Y} - \mathbf{X}\beta)^T (\mathbf{Y} - \mathbf{X}\beta)$ . Maximizing the likelihood is equivalent as minimizing  $(\mathbf{Y} - \mathbf{X}\beta)^T (\mathbf{Y} - \mathbf{X}\beta) = \epsilon^T \epsilon$  which is the SSE.

- Under the assumption of normality, the least-squares coefficients are themselves normally distributed. Summing up,

$$\begin{aligned} \hat{\beta}_0 &\sim N\left(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}\right) \\ \hat{\beta}_1 &\sim N\left(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}\right) \end{aligned}$$

## Statistical inference of the SLR model

Now we have the distribution of  $\hat{\beta}_0$  and  $\hat{\beta}_1$

$$\begin{aligned}\hat{\beta}_0 &\sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}) \\ \hat{\beta}_1 &\sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}).\end{aligned}$$

However,  $\sigma_\epsilon$  is never known in practice. Instead, an *unbiased* estimator of  $\sigma_\epsilon^2$  is given by

$$\hat{\sigma}_\epsilon^2 = MS[E] = \frac{SS[E]}{n-2}.$$

show that  $\mathbf{E}(\sum (y_i - \hat{y}_i)^2) = \sigma_\epsilon^2(n-2)$ .

*Proof:*

$$MS[E] = \frac{\sum (y_i - \hat{y}_i)^2}{n-2},$$

we want to show  $\mathbf{E}(\sum (y_i - \hat{y}_i)^2) = \sigma_\epsilon^2(n-2)$ .

LHS:  $\mathbf{E}(\sum (y_i - \hat{y}_i)^2) = \sum_i [\mathbf{E}(y_i - \hat{y}_i)^2]$

and  $\mathbf{E}[(y_i - \hat{y}_i)^2] = \text{Var}(y_i - \hat{y}_i) + [\mathbf{E}(y_i - \hat{y}_i)]^2 = \text{Var}(y_i - \hat{y}_i) = \text{Var}(y_i) + \text{Var}(\hat{y}_i) - 2\text{cov}(y_i, \hat{y}_i)$

$$\text{Var}(y_i) = \sigma_\epsilon^2$$

$$\text{Var}(\hat{y}_i) = \text{Var}(\bar{y} + \hat{\beta}_1(x_i - \bar{x}))$$

$$= \text{Var}(\bar{y}) + (x_i - \bar{x})^2 \text{Var}(\hat{\beta}_1) + 2(x_i - \bar{x}) \text{Cov}(\bar{y}, \hat{\beta}_1)$$

$$\text{Cov}(\bar{y}, \hat{\beta}_1) = \text{Cov}(\bar{y}, \sum k_i y_i)$$

$$= \sum_i \text{Cov}(\bar{y}, k_i y_i)$$

$$= \sum_i \frac{k_i}{n} \text{Var}(y_i)$$

$$= \frac{1}{n} \sum k_i$$

$$= 0$$

$$\therefore \text{Var}(\hat{y}_i) = \text{Var}(\bar{y}) + (x_i - \bar{x})^2 \text{Var}(\hat{\beta}_1)$$

$$= \frac{1}{n} \sigma_\epsilon^2 + \frac{\sigma_\epsilon^2 (x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2}$$

$$= \sigma_\epsilon^2 \left[ \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right]$$

Now, we derive the last term  $\text{cov}(y_i, \hat{y}_i)$ :

$$\begin{aligned}
\text{cov}(y_i, \hat{y}_i) &= \text{cov}(y_i, \bar{y} + \hat{\beta}_1(x_i - \bar{x})) \\
&= \text{cov}(y_i, \frac{1}{n} \sum_j y_j + (x_i - \bar{x}) \sum_j k_j y_j) \\
&= \text{cov}(y_i, \sum_j \left[ \frac{1}{n} + (x_i - \bar{x})k_j \right] y_j) \\
&= \sigma_\epsilon^2 \left[ \frac{1}{n} + (x_i - \bar{x})k_i \right] \\
&= \sigma_\epsilon^2 \left[ \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right]
\end{aligned}$$

Therefore, we have for  $i$ th residue

$$\begin{aligned}
\text{Var}(y_i - \hat{y}_i) &= \text{Var}(y_i) + \text{Var}(\hat{y}_i) - 2\text{cov}(y_i, \hat{y}_i) \\
&= \sigma_\epsilon^2 + \sigma_\epsilon^2 \left[ \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right] - 2\sigma_\epsilon^2 \left[ \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right] \\
&= \sigma_\epsilon^2 \left[ 1 - \frac{1}{n} - \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right].
\end{aligned}$$

And finally, sum over  $i$  we get

$$\sum_i \text{Var}(y_i - \hat{y}_i) = \sigma_\epsilon^2 \sum_i \left[ 1 - \frac{1}{n} - \frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right] = (n - 2)\sigma_\epsilon^2$$

## Confidence intervals

Now we substitute  $\hat{\sigma}_\epsilon^2$  into the distribution of  $\hat{\beta}_0$  and  $\hat{\beta}_1$

$$\begin{aligned}
\hat{\beta}_1 &\sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}) \\
\hat{\beta}_0 &\sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2})
\end{aligned}$$

to get the estimated standard errors:

$$\begin{aligned}
\widehat{SE}(\hat{\beta}_1) &= \sqrt{\frac{MS[E]}{\sum (x_i - \bar{x})^2}} \\
\widehat{SE}(\hat{\beta}_0) &= \sqrt{MS[E] \left( \frac{1}{n} + \frac{\bar{x}^2}{\sum (x_i - \bar{x})^2} \right)}
\end{aligned}$$

And the  $100(1 - \alpha)\%$  confidence intervals for  $\beta_1$  and  $\beta_0$  are given by

$$\hat{\beta}_1 \pm t(n - 2, \alpha/2) \sqrt{\frac{MS[E]}{S_{xx}}}$$

$$\hat{\beta}_0 \pm t(n-2, \alpha/2) \sqrt{MS[E] \left( \frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)}$$

where  $S_{xx} = \sum (x_i - \bar{x})^2$

**Confidence interval for  $\mathbf{E}(Y|X = x_0)$**

The conditional mean  $\mathbf{E}(Y|X = x_0)$  can be estimated by evaluating the regression function  $\mu(x_0)$  at the estimates  $\hat{\beta}_0, \hat{\beta}_1$ . The conditional variance of the expression isn't too difficult (already shown):

$$\text{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_0 | X = x_0) = \sigma^2 \left( \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)$$

This leads to a confidence interval of the form

$$\hat{\beta}_0 + \hat{\beta}_1 x_0 \pm t(n-2, \alpha/2) \sqrt{MS[E] \left( \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)}$$

**Prediction interval**

Often, prediction of the response variable  $Y$  for a given value, say  $x_0$ , of the independent variable of interest. In order to make statements about future values of  $Y$ , we need to take into account

- the sampling distribution of  $\hat{\beta}_0$  and  $\hat{\beta}_1$
- the randomness of a future value  $Y$ .

We have seen the predicted value of  $Y$  based on the linear regression is given by  $\hat{Y}_0 = \hat{\beta}_0 + \hat{\beta}_1 x_0$ .

The 95% prediction interval has the form

$$\hat{Y}_0 \pm t(n-2, \alpha/2) \sqrt{MS[E] \left( 1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)}.$$

**Hypothesis test**

To test the hypothesis  $H_0 : \beta_1 = \beta_{slope}$  that the population slope is equal to a specific value  $\beta_{slope}$  (most commonly, the null hypothesis has  $\beta_{slope} = 0$ ), we calculate the test statistic ( $T$ -statistics) with  $df = n - 2$

$$t_0 = \frac{\hat{\beta}_1 - \beta_{slope}}{\widehat{SE}(\hat{\beta}_1)} \sim t_{n-2}$$

**Some questions to answer using regression analysis:**

1. What is the meaning, in words, of  $\beta_1$ ?

*Answer:*  $\beta_1$  is the population slope parameter of the SLR model that represents the

amount of increase in the mean of the response variable with a unit increase of the explanatory variable.

2. True/False: (a)  $\beta_1$  is a statistic (b)  $\beta_1$  is a parameter (c)  $\beta_1$  is unknown.

*Answer:* (a) False (b) True (C) True. In reality, the true population parameters are almost never known. However, in simulation studies, we do know them.

3. True/False: (a)  $\hat{\beta}_1$  is a statistic (b)  $\hat{\beta}_1$  is a parameter (c)  $\hat{\beta}_1$  is unknown

*Answer:* (a) True (b) False (C) False.  $\hat{\beta}_1$  is an estimate of the population parameter  $\beta_1$ .

4. Is  $\hat{\beta}_1 = \beta_1$  ?

*Answer:* No. However,  $\mathbf{E}(\hat{\beta}_1) = \beta_1$

## Multiple linear regression

JF 5.2+6.2

### Multiple linear regression - an example

An example on the prestige, education, and income levels of 45 U.S. occupations (Duncan's data):

	income	education	prestige
accountant	62	86	82
pilot	72	76	83
architect	75	92	90
author	55	90	76
chemist	64	86	90
minister	21	84	87
professor	64	93	93
dentist	80	100	90
reporter	67	87	52
engineer	72	86	88
lawyer	76	98	89
teacher	48	91	73

“prestige” represents the percentage of respondents in a survey who rated an occupation as “good” or “excellent” in prestige, “education” represents the percentage of incumbents in the occupation in the 1950 U.S. Census who were high school graduates, and “income” represents the percentage of occupational incumbents who earned incomes in excess of \$3,500.

Using the `pairs` command in R, we can look at the pairwise scatter plot between the three variables as in Figure 12.1.



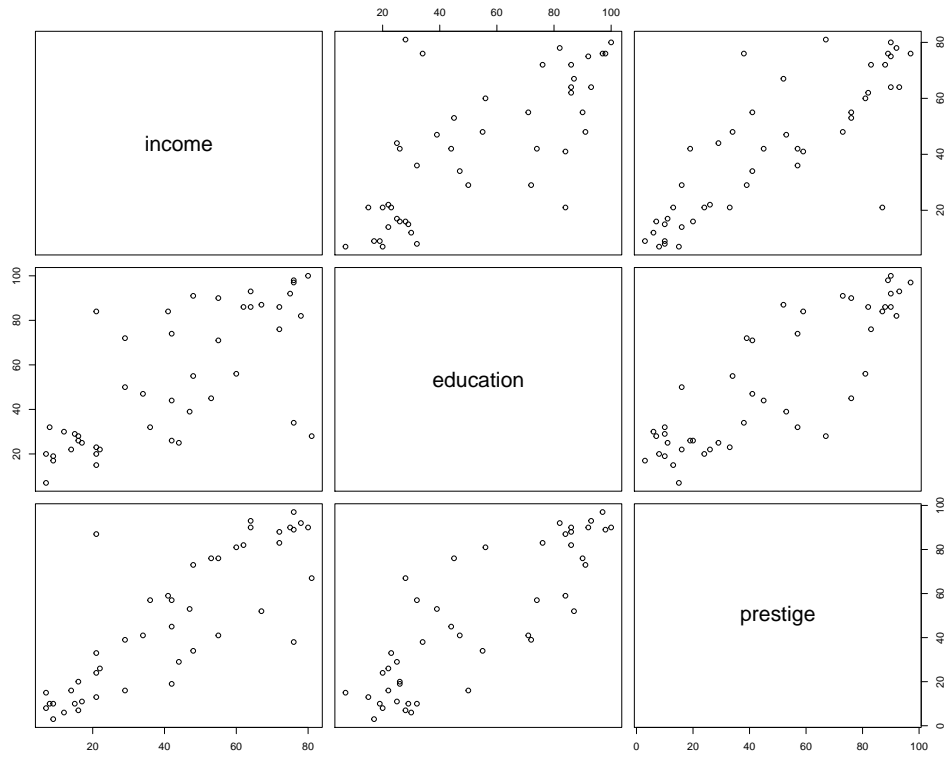


Figure 12.1: Scatterplot matrix for occupational prestige, level of education, and level of income of 45 U.S. occupations in 1950.

Consider a regression model for the “prestige” of occupation  $i$ ,  $Y_i$ , in which the mean of  $Y_i$  is a linear function of two predictor variables  $X_{i1} = \text{income}$ ,  $X_{i2} = \text{education}$  for occupations  $i = 1, 2, \dots, 45$ :

$$Y = \beta_0 + \beta_1 \text{income} + \beta_2 \text{education} + \text{error}$$

or

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i$$

or

$$Y_1 = \beta_0 + \beta_1 X_{11} + \beta_2 X_{12} + \epsilon_1$$

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$$\vdots = \vdots$$

$$Y_{45} = \beta_0 + \beta_1 X_{45,1} + \beta_2 X_{45,2} + \epsilon_{45}$$

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

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

- Observed values of  $p$  independent variables for  $i^{th}$  subject from sample denoted by  $x_{i1}, \dots, x_{ip}$

- response variable for  $i^{th}$  subject denoted by  $Y_i$
- For  $i = 1, \dots, n$ , MLR model for  $Y_i$ :

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

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

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

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

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

Interpretations of regression parameters:

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

## 12 Lecture 14 Feb 22

Last time

- Inference of SLR model

Today

- Confidence intervals for SLR
- Multiple linear regression

### Confidence intervals

Now we substitute  $\hat{\sigma}_\epsilon^2$  into the distribution of  $\hat{\beta}_0$  and  $\hat{\beta}_1$

$$\begin{aligned}\hat{\beta}_1 &\sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum(x_i - \bar{x})^2}) \\ \hat{\beta}_0 &\sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum(x_i - \bar{x})^2})\end{aligned}$$

to get the estimated standard errors:

$$\begin{aligned}\widehat{SE}(\hat{\beta}_1) &= \sqrt{\frac{MS[E]}{\sum(x_i - \bar{x})^2}} \\ \widehat{SE}(\hat{\beta}_0) &= \sqrt{MS[E] \left( \frac{1}{n} + \frac{\bar{x}^2}{\sum(x_i - \bar{x})^2} \right)}\end{aligned}$$

And the  $100(1 - \alpha)\%$  confidence intervals for  $\beta_1$  and  $\beta_0$  are given by

$$\begin{aligned}\hat{\beta}_1 \pm t(n - 2, \alpha/2) \sqrt{\frac{MS[E]}{S_{xx}}} \\ \hat{\beta}_0 \pm t(n - 2, \alpha/2) \sqrt{MS[E] \left( \frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)}\end{aligned}$$

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## Some questions to answer using regression analysis:

1. What is the meaning, in words, of  $\beta_1$ ?  
*Answer:*  $\beta_1$  is the population slope parameter of the SLR model that represents the amount of increase in the mean of the response variable with a unit increase of the explanatory variable.
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## Multiple linear regression

JF 5.2+6.2

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“prestige” represents the percentage of respondents in a survey who rated an occupation as “good” or “excellent” in prestige, “education” represents the percentage of incumbents in the occupation in the 1950 U.S. Census who were high school graduates, and “income” represents the percentage of occupational incumbents who earned incomes in excess of \$3,500.

Using the `pairs` command in R, we can look at the pairwise scatter plot between the three variables as in Figure 12.1.



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Consider a regression model for the “prestige” of occupation  $i$ ,  $Y_i$ , in which the mean of  $Y_i$  is a linear function of two predictor variables  $X_{i1} = \text{income}$ ,  $X_{i2} = \text{education}$  for occupations  $i = 1, 2, \dots, 45$ :

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

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- response variable for  $i^{th}$  subject denoted by  $Y_i$
- For  $i = 1, \dots, n$ , MLR model for  $Y_i$ :

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

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

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

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

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

Interpretations of regression parameters:

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

## Matrix formulation of MLR

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

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

The MLR model for  $Y_1, \dots, Y_n$  is given by

$$\begin{aligned} Y_1 &= \beta_0 + \beta_1 X_{11} + \beta_2 X_{12} + \dots + \beta_p X_{1p} + \epsilon_1 \\ Y_2 &= \beta_0 + \beta_1 X_{21} + \beta_2 X_{22} + \dots + \beta_p X_{2p} + \epsilon_2 \\ &\vdots \\ Y_n &= \beta_0 + \beta_1 X_{n1} + \beta_2 X_{n2} + \dots + \beta_p X_{np} + \epsilon_n \end{aligned}$$

This system of  $n$  equations can be expressed using matrices:

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

where

- $\mathbf{Y}$  denotes a response vector of size  $n \times 1$
- $\mathbf{X}$  denotes a design matrix of size  $n \times (p + 1)$
- $\boldsymbol{\beta}$  denotes a vector of regression parameters of size  $(p + 1) \times 1$

- $\epsilon$  denotes an error vector of size  $n \times 1$

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

$$y_i = \mathbf{x}_i \boldsymbol{\beta} + \epsilon_i.$$

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

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \\ \text{Var}(\hat{\boldsymbol{\beta}}) &= \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1} \\ &= \boldsymbol{\Sigma} \\ \widehat{\text{Var}}(\hat{\boldsymbol{\beta}}) &= MS[E] (\mathbf{X}^T \mathbf{X})^{-1} \\ &= \hat{\boldsymbol{\Sigma}} \\ \widehat{\text{Var}}(\mathbf{a}^T \hat{\boldsymbol{\beta}}) &= \mathbf{a}^T \hat{\boldsymbol{\Sigma}} \mathbf{a}\end{aligned}$$

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

- $(\mathbf{X}^T \mathbf{X})^{-1}$  may be verbalized as “x transposed x inverse”
- $\hat{\boldsymbol{\Sigma}}$  is the estimated variance-covariance matrix for the estimate of the regression parameter vector  $\hat{\boldsymbol{\beta}}$
- $\mathbf{X}$  is assumed to be of full *rank*.

Some more simplified expressions:

$$\begin{aligned}\hat{\mathbf{Y}} &= \mathbf{X} \hat{\boldsymbol{\beta}} \\ &= \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \\ &= \mathbf{H} \mathbf{Y} \\ \hat{\boldsymbol{\epsilon}} &= \mathbf{Y} - \hat{\mathbf{Y}} \\ &= \mathbf{Y} - \mathbf{X} \hat{\boldsymbol{\beta}} \\ &= (\mathbf{I} - \mathbf{H}) \mathbf{Y}\end{aligned}$$

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



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

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

and

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

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

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

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

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

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

### Multiple correlation, JF 5.2.3

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

$$\begin{aligned} TSS &= \sum (Y_i - \bar{Y})^2 \\ RegSS &= \sum (\hat{Y}_i - \bar{Y})^2 \\ RSS &= \sum (Y_i - \hat{Y}_i)^2 = \sum \hat{\epsilon}_i^2 \end{aligned}$$

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

$$TSS = RegSS + RSS$$

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

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

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

## Adjusted- $R^2$

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

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

## Confidence intervals

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

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

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

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

*Hand-waving proof:*

we know that  $t = \frac{\hat{\beta}_i - \beta_i}{\widehat{SE}(\hat{\beta}_i)} \sim t_{n-p-1}$ , such that

$$\begin{aligned} 1 - \alpha &= \Pr(-t_c < t < t_c) \\ &= \Pr\left(t_c < \frac{\hat{\beta}_i - \beta_i}{\widehat{SE}(\hat{\beta}_i)} < t_c\right) \\ &= \Pr\left(\hat{\beta}_i - t_c \cdot \widehat{SE}(\hat{\beta}_i) < \beta_i < \hat{\beta}_i + t_c \cdot \widehat{SE}(\hat{\beta}_i)\right) \end{aligned}$$

where  $t_c = t(n - p - 1, \alpha/2)$  is the critical value.

## Hypothesis tests

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

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

The test statistics,

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

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

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

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

Or more generally, test the null hypothesis

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

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

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

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

4. Find  $p$ -value (the probability of observing an  $F$ -statistic that is at least as high as the value that we obtained) by consulting an  $F$ -distribution with numerator  $df(ndf) = df_{red} - df_{full}$  and denominator  $df(ddf) = df_{full}$ . Notation:  $F_{ndf,ddf}$ , see Figure 12.2.

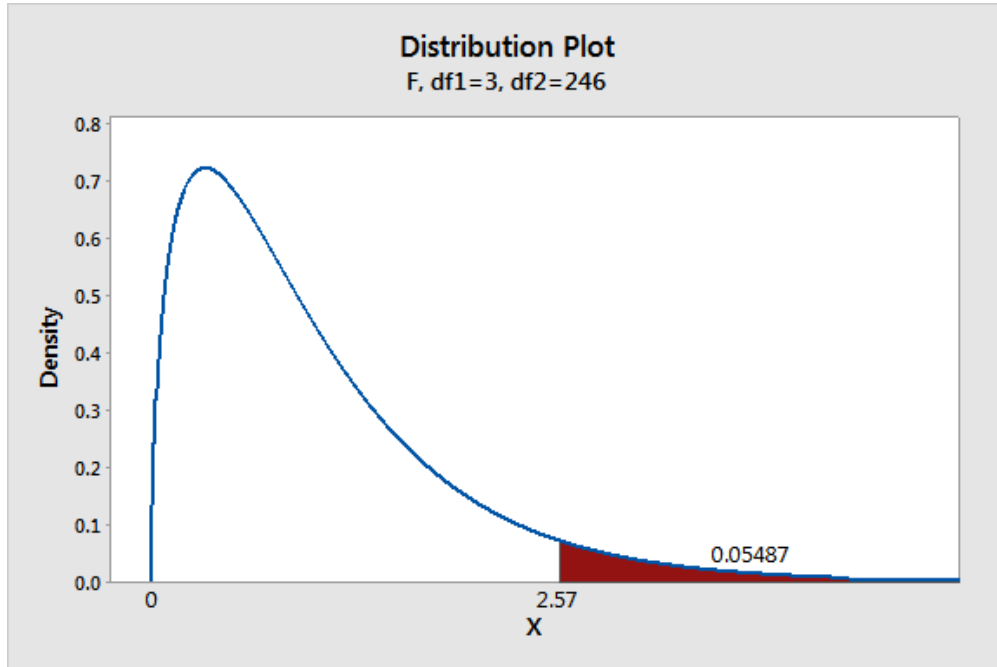


Figure 12.2: An example for  $p$ -value for  $F$ -statistic value 2.57 with an  $F_{3,246}$  distribution