

Multivariate: Matrix algebra

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1 Multivariate

1.1 Goals

1.1.1 Goals of this course

- Familiarize you with **classic** and **modern** multivariate statistics
- Make sure that you understand how to **conduct** these analyses and **interpret** the results
- Prepare you for **further study** in applied statistics
- Give you enough background to **understand** current applied statistics research

1.1.2 Goals of this lecture

- Introduce **matrix algebra**
- Review basic descriptive **statistics**
- Convert expressions for those statistics into **matrix format**

1.2 What is multivariate?

1.2.1 Multivariate?

Variate \approx Variable

Univariate = one variable

Mean, variance

Bivariate = two variables

Correlation between two variables

Multivariate = multiple variables

How several outcomes are related to one another or to predictor(s)

1.2.2 Multivariate?

Multivariate data

- Dataset with many variables
- Typically across many participants
- Often across multiple time points
- “Data cube”

1.2.3 Multivariate?

Multivariate statistics

- Simultaneous analysis of many dependent variables or outcomes
- (There may also be many independent variables or predictors)
- Multivariate analysis is typically accompanied by univariate and bivariate analyses too: means, variances, correlations

1.3 Multivariate techniques

1.3.1 Classic multivariate techniques

Technique	Predictor (IV)	Outcome (DV)
<i>t</i> test	1 discrete, 2 levels	1
One-way ANOVA	1 discrete, >2 levels	1
Factorial ANOVA	≥ 2 discrete	1
Correlation	1 continuous	1
Regression	≥ 2 continuous	1
ANCOVA	Discrete, continuous	1

From Harris, R.N. (1985). A Primer on Multivariate Statistics

1.3.2 Classic multivariate techniques

Technique	Predictor (IV)	Outcome (DV)
Discriminant analysis	1 discrete, 2 levels	≥ 2
MANOVA	1 discrete, >2 levels	≥ 2
Canonical correlation	≥ 2 continuous	≥ 2
PCA	≥ 2 continuous	
FA	≥ 2 continuous	

From Harris, R.N. (1985). A Primer on Multivariate Statistics

1.3.3 Modern multivariate techniques

Models for one outcome variable

- Linear regression, logistic regression, Poisson regression

Models for multiple indicators of a construct

- Factor analysis (FA), principal components analysis (PCA), latent class / profile analysis (LCA / LPA)

Models for multiple outcomes

- Repeated measures ANOVA, MANOVA, mixed models, mediation, path analysis

2 Matrix algebra

2.1 Definitions

2.1.1 Matrix algebra?

Why do we start here?

- Statistics is applied math
- Matrices help us organize a lot of numbers
- Matrix algebra lets us manipulate a lot of numbers at once

Matrix algebra is the language of statistics

2.1.2 Scalar

A scalar is an “ordinary” number

The algebra of scalars is arithmetic

- 4
- $2 + 5 = 7$

2.1.3 Matrix

- **Doubly ordered** arrangement of scalars
 - **Rows** represent one aspect (e.g., subjects)
 - **Columns** represent another (e.g., variables)
- Denoted by capital letters (often **bold** capital letters)
- The **order** (size) of the matrix is ($\#$ rows \times $\#$ columns)
 - In general, matrices are order $p \times q$
- The **elements** in the matrix are identified by subscripts
 - Element a_{ij} is in row i and column j

2.1.4 Matrix **X** with 4 rows and 3 columns

$$\begin{matrix} \mathbf{X} \\ (4, 3) \end{matrix} = \begin{bmatrix} 2 & 6 & 5 \\ 8 & 1 & 4 \\ 9 & 3 & 6 \\ 2 & 0 & 5 \end{bmatrix}$$

2.1.5 Matrix **A** with 2 rows and 5 columns

$$\begin{matrix} \mathbf{A} \\ (2, 5) \end{matrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \end{bmatrix}$$

2.1.6 Vector

- A **row vector** is a matrix of order $1 \times q$
- A **column vector** is a matrix of order $p \times 1$
- Denoted by lower case, underlined letters

2.1.7 Row vector

$$\underline{x}_{(1,q)} = [x_1 \quad x_2 \quad \cdots \quad x_q]$$

2.1.8 Column vector

$$\underline{y}_{(p,1)} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

2.2 Matrix algebra

2.2.1 Matrix algebra

Matrix algebra is the set of rules for performing mathematical operations on matrices (and vectors)

- Addition and subtraction are straight-forward extensions
- Multiplication and division are not
- Other matrix-specific operations, such as the transpose

2.2.2 Transpose

- Switch the rows and columns
- Rows become columns and columns become rows

$$\begin{matrix} \mathbf{A} \\ (2,3) \end{matrix} = \begin{bmatrix} 6 & 2 & 4 \\ 8 & 1 & 0 \end{bmatrix}$$

$$\begin{matrix} \mathbf{A}' \\ (3,2) \end{matrix} = \begin{matrix} \mathbf{A}^T \\ (3,2) \end{matrix} = \begin{bmatrix} 6 & 8 \\ 2 & 1 \\ 4 & 0 \end{bmatrix}$$

2.2.3 Transpose

- The transpose of a column vector is a row vector
- The transpose of a row vector is a column vector

$$\begin{matrix} \underline{x} \\ (4,1) \end{matrix} = \begin{bmatrix} 2 \\ 8 \\ 9 \\ 2 \end{bmatrix}$$

$$\begin{matrix} \underline{x}' \\ (1,4) \end{matrix} = \begin{matrix} \underline{x}^T \\ (1,4) \end{matrix} = \begin{bmatrix} 2 & 8 & 9 & 2 \end{bmatrix}$$

2.2.4 Addition

Matrices must be of the **same order** to be **conformable** for addition

- $\mathbf{A} + \mathbf{B} = \mathbf{C}$
- Add corresponding elements: $c_{ij} = a_{ij} + b_{ij}$

$$\begin{bmatrix} 3 & 1 & 5 \\ 2 & 4 & 6 \end{bmatrix} + \begin{bmatrix} 2 & 4 & 7 \\ 8 & 11 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 5 & 12 \\ 10 & 15 & 10 \end{bmatrix}$$

- Commutative: $(\mathbf{A} + \mathbf{B}) = (\mathbf{B} + \mathbf{A})$
- Associative: $[\mathbf{A} + (\mathbf{B} + \mathbf{C})] = [(\mathbf{A} + \mathbf{B}) + \mathbf{C}]$

2.2.5 Subtraction

Matrices must be of the **same order** to be **conformable** for subtraction

- $\mathbf{A} - \mathbf{B} = \mathbf{D}$
- Add corresponding elements: $d_{ij} = a_{ij} - b_{ij}$

$$\begin{bmatrix} 3 & 1 & 5 \\ 2 & 4 & 6 \end{bmatrix} - \begin{bmatrix} 2 & 4 & 7 \\ 8 & 11 & 4 \end{bmatrix} = \begin{bmatrix} 1 & -3 & -2 \\ -6 & -7 & 2 \end{bmatrix}$$

2.2.6 Multiplication

- Multiplication of matrices is more complicated
- This is “inner” or “dot” product matrix multiplication
 - There is also an “outer” product, which we won’t use

Rules for matrix multiplication

- $\begin{matrix} \mathbf{A} & \mathbf{B} \\ (p,q) & (q,r) \end{matrix} = \begin{matrix} \mathbf{C} \\ (p,r) \end{matrix}$
- $c_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + \dots + a_{ip}b_{pj} = \sum a_{ik}b_{kj}$

2.2.7 Multiplication example: matrix times matrix

$$\begin{matrix} \mathbf{A} & \mathbf{B} \\ (2,3) & (3,2) \end{matrix} = \begin{matrix} \mathbf{C} \\ (2,2) \end{matrix}$$

$$\begin{bmatrix} 2 & 4 & 1 \\ 3 & 0 & 4 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 0 \\ 4 & 2 \end{bmatrix} = \begin{bmatrix} 14 & 8 \\ 19 & 17 \end{bmatrix}$$

Row 1, Column 1: $(2 \times 1) + (4 \times 2) + (1 \times 4) = 14$

Row 1, Column 2: $(2 \times 3) + (4 \times 0) + (1 \times 2) = 8$

Row 2, Column 1: $(3 \times 1) + (0 \times 2) + (4 \times 4) = 19$

Row 2, Column 2: $(3 \times 3) + (0 \times 0) + (4 \times 2) = 17$

2.2.8 Multiplication example: matrix times column vector

$$\begin{matrix} \text{A} & \underline{b} \\ (2,3) & (3,1) \end{matrix} = \begin{matrix} \underline{c} \\ (2,1) \end{matrix}$$

$$\begin{bmatrix} 2 & 4 & 1 \\ 3 & 0 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 14 \\ 19 \end{bmatrix}$$

Row 1, Column 1: $(2 \times 1) + (4 \times 2) + (1 \times 4) = 14$

Row 2, Column 1: $(3 \times 1) + (0 \times 2) + (4 \times 4) = 19$

2.2.9 Multiplication example: data matrix times column vector of regression coefficients

$$\begin{matrix} \mathbf{X} & \underline{b} \\ (5,3) & (3,1) \end{matrix} = \begin{matrix} \underline{c} \\ (5,1) \end{matrix}$$

$$\begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \\ X_{41} & X_{42} & X_{43} \\ X_{51} & X_{52} & X_{53} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} b_1 X_{11} + b_2 X_{12} + b_3 X_{13} \\ b_1 X_{21} + b_2 X_{22} + b_3 X_{23} \\ b_1 X_{31} + b_2 X_{32} + b_3 X_{33} \\ b_1 X_{41} + b_2 X_{42} + b_3 X_{43} \\ b_1 X_{51} + b_2 X_{52} + b_3 X_{53} \end{bmatrix}$$

2.2.10 Multiplication example: row vector times column vector

$$\begin{matrix} \underline{a'} & \underline{b} \\ (1,3) & (3,1) \end{matrix} = \begin{matrix} \underline{c} \\ (1,1) \end{matrix}$$

$$\begin{bmatrix} 3 & 1 & 5 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 9 \end{bmatrix} = [55]$$

$(3 \times 2) + (1 \times 4) + (5 \times 9) = 55$

2.2.11 Multiplication example: column vector times row vector

$$\begin{matrix} \underline{b} & \underline{a'} \\ (3,1) & (1,3) \end{matrix} = \begin{matrix} \mathbf{C} \\ (3,3) \end{matrix}$$

$$\begin{bmatrix} 2 \\ 4 \\ 9 \end{bmatrix} \begin{bmatrix} 3 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 6 & 2 & 10 \\ 12 & 4 & 20 \\ 27 & 9 & 45 \end{bmatrix}$$

Row 1, Column 1: $(2 \times 3) = 6$

Row 1, Column 2: $(2 \times 1) = 2$

Row 1, Column 3: $(2 \times 5) = 10$

Row 2, Column 1: $(4 \times 3) = 12$

Row 2, Column 2: $(4 \times 1) = 4$

Row 2, Column 3: $(4 \times 5) = 20$

Row 3, Column 1: $(9 \times 3) = 27$

Row 3, Column 2: $(9 \times 1) = 9$

Row 3, Column 3: $(9 \times 5) = 45$

2.2.12 Multiplication example: matrix times a scalar

Multiply every element in the matrix by the scalar

$$3 \times \begin{bmatrix} 3 & 2 & 4 \\ 1 & 2 & 3 \\ 8 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 9 & 6 & 12 \\ 3 & 6 & 9 \\ 24 & 3 & 3 \end{bmatrix}$$

2.2.13 Multiplication of matrices: Associative

$$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$$

- When multiplying > 2 matrices, it doesn't matter which two you start with
- Must keep the same overall order

2.2.14 Multiplication of matrices: Distributive

With respect to addition and subtraction:

$$\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}$$

- Distribute the \mathbf{A} matrix as you would in arithmetic

2.2.15 Multiplication of matrices: NOT commutative

$$\mathbf{AB} \neq \mathbf{BA}$$

- **Order matters for matrix multiplication**
- See *row \times column* and *column \times row* examples

2.2.16 Multiplication of matrices: Transpose and multiplication

- If $\mathbf{D} = \mathbf{AB}$, then $\mathbf{D}' = \mathbf{B}'\mathbf{A}'$
 - The transpose is equal to the product of the transposes in **reverse order**

2.2.17 Division

Division is not defined for matrices

Instead of dividing, we **multiply by the inverse**

- The inverse of a number is the number raised to the power of -1
 - e.g., inverse of 5 = $5^{-1} = \frac{1}{5}$

We do the same in regular arithmetic:

- Divide: $30/5 = 6$
- Multiply by inverse: $30 \times 5^{-1} = 30 \times \frac{1}{5} = 6$

2.2.18 Division

Calculating the inverse of a matrix is complicated (more later)

Multiplying the matrix by its inverse results in the **identity matrix**:

$$\mathbf{A} \mathbf{A}^{-1} = \mathbf{A}^{-1} \mathbf{A} = \mathbf{I}$$

2.2.19 Identity matrix

The identity matrix (**I**) is a special matrix that looks like:

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

1s on the **main diagonal**, 0s elsewhere

Multiplying a matrix by **I** is like multiplying it by 1

- Why would you do this? To be able to perform other matrix operations

2.2.20 Matrix times inverse = identity matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 4 & 1 \end{bmatrix} \quad \mathbf{A}^{-1} = \begin{bmatrix} 1 & -2 & 1 \\ -\frac{3}{5} & 1 & -\frac{1}{5} \\ \frac{2}{5} & 0 & -\frac{1}{5} \end{bmatrix}$$

$$\text{Row 1, Column 1: } 1 = (1 \times 1) + (2 \times -\frac{3}{5}) + (3 \times \frac{2}{5})$$

$$\text{Row 1, Column 2: } 0 = (1 \times -2) + (2 \times 1) + (3 \times 0)$$

$$\text{Row 1, Column 3: } 0 = (1 \times 1) + (2 \times -\frac{1}{5}) + (3 \times -\frac{1}{5})$$

$$\text{Row 2, Column 1: } 0 = (1 \times 1) + (3 \times -\frac{3}{5}) + (2 \times \frac{2}{5})$$

$$\text{Row 2, Column 2: } 1 = (1 \times -2) + (3 \times 1) + (2 \times 0)$$

$$\text{Row 2, Column 3: } 0 = (1 \times 1) + (3 \times -\frac{1}{5}) + (2 \times -\frac{1}{5})$$

$$\text{Row 3, Column 1: } 0 = (2 \times 1) + (4 \times -\frac{3}{5}) + (1 \times \frac{2}{5})$$

$$\text{Row 3, Column 2: } 0 = (2 \times -2) + (4 \times 1) + (1 \times 0)$$

$$\text{Row 3, Column 3: } 1 = (2 \times 1) + (4 \times -\frac{1}{5}) + (1 \times -\frac{1}{5})$$

3 Review: Basic statistics

3.1 Statistics

This section **reviews** material you should already be familiar with from previous courses

You don't need to memorize these equations, but you should be *comfortable* with using them

All of the material in this course (and in all of statistics!) builds on these basic concepts of *central tendency*, *variability*, and *covariability*

3.2 Central tendency

3.2.1 Arithmetic mean

- **Population:**

$$\mu_X = \frac{\sum X}{N}$$

where N is the size of the *population*

- **Sample:**

$$\bar{X} = \frac{\sum X}{n}$$

where n is the size of the *sample*

3.3 Variability of one variable

3.3.1 Variation

Sum of squared deviations from mean: sum of squares (SS)

- **Population:**

$$SS_X = \sum (X_i - \mu_X)^2 = \sum X^2 - \frac{(\sum X)^2}{N}$$

where μ_X is the *population* mean

- **Sample:**

$$SS_X = \sum (X_i - \bar{X})^2 = \sum X^2 - \frac{(\sum X)^2}{n}$$

where \bar{X} is the *sample* mean

3.3.2 Variance

Average squared deviation of scores around the mean

- **Population:**

$$\sigma^2_X = \frac{\sum (X_i - \mu_X)^2}{N} = \frac{\sum X^2 - \frac{(\sum X)^2}{N}}{N}$$

where μ_X is the *population* mean and N is the *population* size

- **Sample:**

$$s^2_X = \frac{\sum (X_i - \bar{X})^2}{n-1} = \frac{\sum X^2 - \frac{(\sum X)^2}{n}}{n-1}$$

where \bar{X} is the *sample* mean and n is the *sample* size

3.3.3 Standard deviation

Square root of variance: in the same units as the original variable

- **Population:**

$$\sigma_X = \sqrt{\frac{\sum (X_i - \mu_X)^2}{N}} = \sqrt{\frac{\sum X^2 - \frac{(\sum X)^2}{N}}{N}}$$

- **Sample:**

$$s_X = \sqrt{\frac{\sum (X_i - \bar{X})^2}{n-1}} = \sqrt{\frac{\sum X^2 - \frac{(\sum X)^2}{n}}{n-1}}$$

3.4 Relationship between 2 variables

3.4.1 Covariation

Analogous to **variation**: *sum of cross-products* of the deviations or sum of products (SP)

- **Population:**

$$SP_{XY} = \sum (X_i - \mu_X)(Y_i - \mu_Y) = \sum XY - \frac{(\sum X)(\sum Y)}{N}$$

where μ_X and μ_Y are the *population* means

- **Sample:**

$$SP_{XY} = \sum (X_i - \bar{X})(Y_i - \bar{Y}) = \sum XY - \frac{(\sum X)(\sum Y)}{n}$$

where \bar{X} and \bar{Y} are the *sample* means

3.4.2 Covariance

Analogous to **variance**: *average* sum of cross-products of the deviations around the mean

- **Population:**

$$\sigma_{XY} = \frac{\sum (X_i - \mu_X)(Y_i - \mu_Y)}{N} = \frac{\sum XY - \frac{(\sum X)(\sum Y)}{N}}{N}$$

- **Sample:**

$$s_{XY} = \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{n-1} = \frac{\sum XY - \frac{(\sum X)(\sum Y)}{n}}{n-1}$$

3.4.3 Correlation

Standardized measure of how two variables are related

- **Population:**

$$\rho_{XY} = \frac{\sum z_X z_Y}{N} = \frac{SP_{XY}}{\sqrt{SS_X} \sqrt{SS_Y}} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y}$$

- **Sample:**

$$r_{XY} = \frac{\sum z_X z_Y}{n} = \frac{SP_{XY}}{\sqrt{SS_X} \sqrt{SS_Y}} = \frac{s_{XY}}{s_X s_Y}$$

where z_X and z_Y are standard scores (z -scores):

$$z_X = \frac{X_i - \mu_X}{\sigma_X} \text{ (population) or } z_X = \frac{X_i - \bar{X}}{s_X} \text{ (sample)}$$

4 Basic statistics: Matrix!

4.1 Data matrix

4.1.1 Data matrix

Data is usually presented as

- Rows for subjects
- Columns for variables

The *data matrix* is an $n \times p$ matrix

- n subjects (rows: $1, 2, \dots, i, \dots, n$)
- p variables (columns: $X_1, X_2, \dots, X_j, \dots, X_p$)

4.1.2 Data matrix

$$\mathbf{X} = \begin{bmatrix} X_{11} & \cdots & X_{1j} & \cdots & X_{1p} \\ \vdots & & \vdots & & \vdots \\ X_{i1} & \cdots & X_{ij} & \cdots & X_{ip} \\ \vdots & & \vdots & & \vdots \\ X_{n1} & \cdots & X_{nj} & \cdots & X_{np} \end{bmatrix}$$

4.2 Unit vector and matrix

4.2.1 Unit vector

The unit vector is a vector filled with 1s

$$\underline{1}_{(n,1)} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

- Used to **add numbers in a matrix together**
- Same function as \sum in arithmetic: $\sum_{i=1}^n X = \underline{1}' \underline{x}$
- The unit vector $\underline{1}$ is typically a *column vector* but we can also use its transpose $\underline{1}'$ when we need a *row vector*

4.2.2 Unit vector adds up elements

$$\underline{1}'_{(1,4)} = [1 \quad 1 \quad 1 \quad 1] \quad \underline{x}_{(4,1)} = \begin{bmatrix} 4 \\ 3 \\ 8 \\ 2 \end{bmatrix}$$

$$\underline{1}' \underline{x} = (1 \times 4) + (1 \times 3) + (1 \times 8) + (1 \times 2) =$$

$$4 + 3 + 8 + 2 = 17$$

4.2.3 Unit matrix

The unit matrix is a matrix filled with 1s

$$\mathbf{E}_{(n,n)} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

- Used to **add numbers** and **create products of numbers**
- For most of our purposes, we'll use an $n \times n$ version, but it can be any size / order

4.3 Central tendency

4.3.1 Mean of a single variable

Pre-multiply the vector of values by the unit vector and multiply by inverse of n

$$\bar{X} = \frac{1}{n} \underline{1}' \underline{x}$$

4.3.2 Mean of a single variable

Example: Variable X is observed for $n = 4$ subjects

$$\begin{matrix} \underline{1}' \\ (1,4) \end{matrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} \begin{matrix} \underline{x} \\ (4,1) \end{matrix} = \begin{bmatrix} 4 \\ 3 \\ 8 \\ 2 \end{bmatrix}$$

$$\bar{X} = \frac{1}{n} \underline{1}' \underline{x} =$$

$$\frac{1}{4}[(1 \times 4) + (1 \times 3) + (1 \times 8) + (1 \times 2)] =$$

$$\frac{1}{4}(4 + 3 + 8 + 2) = \frac{17}{4} = 4.25$$

4.3.3 Mean of several variables

Example: Variables X_1 , X_2 , and X_3 for $n = 4$ subjects

$$\begin{matrix} \underline{1}' \\ (1,4) \end{matrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} \begin{matrix} \mathbf{X} \\ (4,3) \end{matrix} = \begin{bmatrix} 4 & 2 & 4 \\ 3 & 1 & 1 \\ 8 & 3 & 2 \\ 2 & 5 & 5 \end{bmatrix}$$

$$\underline{\bar{x}} = \frac{1}{n} \underline{1}' \mathbf{X} = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 4 & 2 & 4 \\ 3 & 1 & 1 \\ 8 & 3 & 2 \\ 2 & 5 & 5 \end{bmatrix} =$$

$$\frac{1}{4} [4 + 3 + 8 + 2 \quad 2 + 1 + 3 + 5 \quad 4 + 1 + 2 + 5] =$$

$$\frac{1}{4} [17 \quad 11 \quad 12] = [4.25 \quad 2.75 \quad 3]$$

4.4 (Co)variation

4.4.1 Some matrix algebra properties

Sum a variable across all subjects:

$$\sum X = \sum_{i=1}^n X = \underline{1}' \mathbf{X} = \mathbf{X}' \underline{1}$$

Sum THEN square:

$$(\sum X)^2 = (\sum_{i=1}^n X)^2 = \mathbf{X}' \underline{1} \underline{1}' \mathbf{X} = \mathbf{X}' \mathbf{E} \mathbf{X}$$

Square THEN sum:

$$\sum(X^2) = \sum_{i=1}^n (X^2) = \mathbf{X}' \mathbf{X}$$

4.4.2 Variation

Recall that the *sample variation* is:

$$SS_X = \sum (X_i - \bar{X})^2 = \sum (X^2) - \frac{(\sum X)^2}{n}$$

4.4.3 Variation

Recall that the *sample variation* is:

$$SS_X = \sum (X_i - \bar{X})^2 = \sum (X^2) - \frac{(\sum X)^2}{n}$$

And that:

$$\sum(X^2) = \mathbf{X}' \mathbf{X}$$

$$(\sum X)^2 = \mathbf{X}' \underline{1} \underline{1}' \mathbf{X} = \mathbf{X}' \mathbf{E} \mathbf{X}$$

4.4.4 Variation

Recall that the *sample variation* is:

$$SS_X = \sum (X_i - \bar{X})^2 = \sum (X^2) - \frac{(\sum X)^2}{n}$$

And that:

$$\sum (X^2) = \mathbf{X}' \mathbf{X}$$

$$(\sum X)^2 = \mathbf{X}' \mathbf{1} \mathbf{1}' \mathbf{X} = \mathbf{X}' \mathbf{E} \mathbf{X}$$

Substitute matrix expressions:

$$SS_X = \mathbf{X}' \mathbf{X} - \frac{1}{n} (\mathbf{X}' \mathbf{E} \mathbf{X})$$

4.4.5 Covariation

Recall that the *sample covariation* is:

$$SP_{XY} = \sum (X_i - \bar{X})(Y_i - \bar{Y}) = \sum XY - \frac{(\sum X)(\sum Y)}{n}$$

4.4.6 Covariation

Recall that the *sample covariation* is:

$$SP_{XY} = \sum (X_i - \bar{X})(Y_i - \bar{Y}) = \sum XY - \frac{(\sum X)(\sum Y)}{n}$$

And that (extending to the X and Y situation):

$$\sum (XY) = \mathbf{X}' \mathbf{Y}$$

$$(\sum X)(\sum Y) = \mathbf{X}' \mathbf{1} \mathbf{1}' \mathbf{Y} = \mathbf{X}' \mathbf{E} \mathbf{Y}$$

4.4.7 Covariation

Recall that the *sample covariation* is:

$$SP_{XY} = \sum (X_i - \bar{X})(Y_i - \bar{Y}) = \sum XY \frac{(\sum X)(\sum Y)}{n}$$

And that (extending to the X and Y situation):

$$\sum(XY) = \mathbf{X}' \mathbf{Y}$$

$$(\sum X)(\sum Y) = \mathbf{X}' \mathbf{1} \mathbf{1}' \mathbf{Y} = \mathbf{X}' \mathbf{E} \mathbf{Y}$$

Substitute matrix expressions:

$$SP_{XY} = \mathbf{X}' \mathbf{Y} - \frac{1}{n} (\mathbf{X}' \mathbf{E} \mathbf{Y})$$

4.4.8 Variation-covariation matrix (\mathbf{P})

- Involves many variables
- Subscripts indicate which variables are involved: \mathbf{P}_{XX} , \mathbf{P}_{XY}
- **Variation** along the diagonal, **covariation** elsewhere

$$\mathbf{P}_{XX} = \mathbf{X}' \mathbf{X} - \frac{1}{n} \mathbf{X}' \mathbf{E} \mathbf{X} = \begin{bmatrix} \textcolor{blue}{SS}_{X_1} & SP_{X_1 X_2} & \cdots & SP_{X_1 X_p} \\ SP_{X_2 X_1} & \textcolor{blue}{SS}_{X_2} & \cdots & SP_{X_2 X_p} \\ \vdots & \vdots & \ddots & \vdots \\ SP_{X_p X_1} & SP_{X_p X_2} & \cdots & \textcolor{blue}{SS}_{X_p} \end{bmatrix}$$

4.5 (Co)variance

4.5.1 Variance

Recall that the *sample variance* is:

$$s_X^2 = \frac{\text{variation}}{n-1} = \frac{SS_X}{n-1}$$

Multiply the matrix expression for variation by $\frac{1}{n-1}$:

$$s_X^2 = \frac{1}{n-1} \left(\mathbf{X}' \mathbf{X} - \frac{1}{n} (\mathbf{X}' \mathbf{E} \mathbf{X}) \right)$$

4.5.2 Covariance

Recall that the *sample covariance* is:

$$\text{cov}_{XY} = s_{XY} = \frac{\text{covariation}}{n-1} = \frac{SP_{XY}}{n-1}$$

Multiply the matrix expression for covariation by $\frac{1}{n-1}$:

$$\text{cov}_{XY} = s_{XY} = \frac{1}{n-1} \left(\mathbf{X}' \mathbf{Y} - \frac{1}{n} (\mathbf{X}' \mathbf{E} \mathbf{Y}) \right)$$

4.5.3 Variance-covariance matrix (S)

- Involves many variables
- Subscripts indicate which variables are involved: \mathbf{S}_{XX} , \mathbf{S}_{XY}
- **Variance** along the diagonal, **covariance** elsewhere
- **One of THE most important matrices in statistics**

$$\mathbf{S}_{XX} = \frac{1}{n-1} (\mathbf{X}' \mathbf{X} - \frac{1}{n} \mathbf{X}' \mathbf{E} \mathbf{X}) = \begin{bmatrix} s_{X_1}^2 & s_{X_1 X_2} & \cdots & s_{X_1 X_p} \\ s_{X_2 X_1} & s_{X_2}^2 & \cdots & s_{X_2 X_p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{X_p X_1} & s_{X_p X_2} & \cdots & s_{X_p}^2 \end{bmatrix}$$

4.6 Correlation

4.6.1 Correlation

The correlation between X and Y is:

$$r_{XY} = \frac{SP_{XY}}{\sqrt{SS_X}\sqrt{SS_Y}}$$

Since division for matrices means **multiplication by the inverse**:

- We need the inverse of $\sqrt{SS_X}$ and $\sqrt{SS_Y}$
- i.e., $\sqrt{SS_X}^{-1}$ and $\sqrt{SS_Y}^{-1}$

4.6.2 Reciprocals of square root of variation

\mathbf{D}_P is a matrix with the square root of **variation** on the diagonal:

$$\mathbf{D}_P = \begin{bmatrix} \sqrt{SS_{X_1}} & 0 & \cdots & 0 \\ 0 & \sqrt{SS_{X_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{SS_{X_p}} \end{bmatrix}$$

The inverse of \mathbf{D}_P :

$$\mathbf{D}_P^{-1} = \begin{bmatrix} \frac{1}{\sqrt{SS_{X_1}}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{SS_{X_2}}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{SS_{X_p}}} \end{bmatrix}$$

4.6.3 Reciprocals of square root of variance

\mathbf{D}_S is a matrix with the square root of **variance** on the diagonal:

$$\mathbf{D}_S = \begin{bmatrix} \sqrt{s_{X_1}^2} & 0 & \cdots & 0 \\ 0 & \sqrt{s_{X_2}^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{s_{X_p}^2} \end{bmatrix}$$

The inverse of \mathbf{D}_S :

$$\mathbf{D}_S^{-1} = \begin{bmatrix} \frac{1}{\sqrt{s_{X_1}^2}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{s_{X_2}^2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{s_{X_p}^2}} \end{bmatrix}$$

4.6.4 Correlation matrix (\mathbf{R})

- Involves many variables
- Subscripts indicate which variables are involved: \mathbf{R}_{XX} , \mathbf{R}_{XY}
- 1s along the diagonal, **correlations** elsewhere
- **One of THE most important matrices in statistics**

4.6.5 Correlation matrix (\mathbf{R})

In terms of *variation and covariation*:

$$\mathbf{R}_{XX} = \mathbf{D}_P^{-1} \mathbf{P} \mathbf{D}_P^{-1} = \begin{bmatrix} 1 & r_{X_1 X_2} & \cdots & r_{X_1 X_p} \\ r_{X_2 X_1} & 1 & \cdots & r_{X_2 X_p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{X_p X_1} & r_{X_p X_2} & \cdots & 1 \end{bmatrix}$$

4.6.6 Correlation matrix (**R**)

In terms of *variance and covariance*:

$$\mathbf{R}_{XX} = \mathbf{D}_S^{-1} \mathbf{S} \mathbf{D}_S^{-1} = \begin{bmatrix} 1 & r_{X_1 X_2} & \cdots & r_{X_1 X_p} \\ r_{X_2 X_1} & 1 & \cdots & r_{X_2 X_p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{X_p X_1} & r_{X_p X_2} & \cdots & 1 \end{bmatrix}$$