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)
t 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 MANOVA	1 discrete, 2 levels 1 discrete, >2 levels	≥ 2 > 2
Canonical correlation	≥ 2 continuous	≥ 2
PCA FA	≥ 2 continuous ≥ 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 × # 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

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

2.1.5 Matrix A with 2 rows and 5 columns

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

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

$$\frac{\underline{x}}{(1,q)} = \begin{bmatrix} x_1 & x_2 & \cdots & x_q \end{bmatrix}$$

2.1.8 Column vector

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

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

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

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

2.2.3 Transpose

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

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

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

2.2.4 Addition

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

•
$$\mathbf{A} + \mathbf{B} = \mathbf{C}$$

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

- 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

- A B = 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

•
$$\frac{\mathbf{A}}{(p,q)} \times \frac{\mathbf{B}}{(q,r)} = \frac{\mathbf{C}}{(p,r)}$$

•
$$c_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + \dots + a_{ip}b_{pj} = \sum a_{ik}b_{kj}$$

2.2.7 Multiplication example: matrix times matrix

$$\mathbf{A} \quad \mathbf{B} \\ \mathbf{(2,3)} \quad \mathbf{(3,2)} = \mathbf{C} \\ \mathbf{(2,2)}$$

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

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

$$\frac{\mathbf{A}}{(2,3)} \frac{\underline{b}}{(3,1)} = \frac{\underline{c}}{(2,1)}$$

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

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

$$\frac{\mathbf{X}}{(5,3)} \frac{\underline{b}}{(3,1)} = \frac{\underline{c}}{(5,1)}$$

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

2.2.10 Multiplication example: row vector times column vector

$$\frac{\underline{a'}}{(1,3)} \frac{\underline{b}}{(3,1)} = \frac{\underline{c}}{(1,1)}$$

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

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

2.2.11 Multiplication example: column vector times row vector

$$\frac{\underline{b}}{(3,1)} \frac{\underline{a'}}{(1,3)} = \mathbf{C}$$

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

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

 $(\mathbf{A}\mathbf{B})\mathbf{C} = \mathbf{A}(\mathbf{B}\mathbf{C})$

- 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:

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

• Distribute the A matrix as you would in arithmetic

2.2.15 Multiplication of matrices: NOT commutative

 $AB \neq BA$

- Order matters for matrix multiplication
- See $row \ x \ column \ and \ column \ x \ row \ examples$

2.2.16 Multiplication of matrices: Transpose and multiplication

• If D = AB, then D' = B'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 (\mathbf{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 ${\bf I}$ is like multiplying it by 1

 $\bullet\,$ Why would you do this? To be able to perform other matrix operations

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2.2.20 Matrix times inverse = identity matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 4 & 1 \end{bmatrix} \qquad \mathbf{A}^{-1} = \begin{bmatrix} 1 & -2 & 1 \\ -\frac{3}{5} & 1 & -\frac{1}{5} \\ \frac{2}{5} & 0 & -\frac{1}{5} \end{bmatrix}$$
Row 1, Column 1:
$$1 = (1 \times 1) + (2 \times -\frac{3}{5}) + (3 \times \frac{2}{5})$$
Row 1, Column 2:
$$0 = (1 \times -2) + (2 \times 1) + (3 \times 0)$$
Row 1, Column 3:
$$0 = (1 \times 1) + (2 \times -\frac{1}{5}) + (3 \times -\frac{1}{5})$$
Row 2, Column 1:
$$0 = (1 \times 1) + (3 \times -\frac{3}{5}) + (2 \times \frac{2}{5})$$
Row 2, Column 2:
$$1 = (1 \times -2) + (3 \times 1) + (2 \times 0)$$
Row 2, Column 3:
$$0 = (1 \times 1) + (3 \times -\frac{1}{5}) + (2 \times -\frac{1}{5})$$
Row 3, Column 1:
$$0 = (2 \times 1) + (4 \times -\frac{3}{5}) + (1 \times \frac{2}{5})$$
Row 3, Column 2:
$$1 = (2 \times 1) + (4 \times -\frac{1}{5}) + (1 \times -\frac{1}{5})$$
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

3.1.1 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:

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

where N is the size of the population

• Sample:

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

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:

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

where \overline{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:

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

where \overline{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:

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

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:

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

where \overline{X} and \overline{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:

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

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):

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

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

- 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 us its transpose $\underline{1}'$ when we need a *row vector*

4.2.2 Unit vector adds up elements

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

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

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

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

4.3.2 Mean of a single variable

Example: Variable X is observed for n = 4 subjects

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

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

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

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

4.3.3 Mean of several variables

Example: Variables $X_1,\,X_2,\,{\rm and}\,\,X_3$ for n=4 subjects

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

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

$$\frac{1}{4} \begin{bmatrix} 4+3+8+2 & 2+1+3+5 & 4+1+2+5 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 17 & 11 & 12 \end{bmatrix} = \begin{bmatrix} 4.25 & 2.75 & 3 \end{bmatrix}$$

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:

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

4.4.3 Variation

Recall that the *sample variation* is:

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

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:

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

And that:

$$\begin{split} & \sum (X^2) = \mathbf{X}' \; \mathbf{X} \\ & (\sum X)^2 = \mathbf{X}' \; \underline{1} \; \underline{1}' \; \mathbf{X} = \mathbf{X}' \; \mathbf{E} \; \mathbf{X} \end{split}$$

Substitute matrix expressions:

$$SS_X = \textbf{X}' \ \textbf{X} - \frac{1}{n} \left(\textbf{X}' \ \textbf{E} \ \textbf{X} \right)$$

4.4.5 Covariation

Recall that the *sample covariation* is:

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

4.4.6 Covariation

Recall that the *sample covariation* is:

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

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

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

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

4.4.7 Covariation

Recall that the *sample covariation* is:

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

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

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

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

Substitute matrix expressions:

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

4.4.8 Variation-covariation matrix (P)

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

$$\mathbf{P}_{XX} = \mathbf{X'X} - \frac{1}{n}\mathbf{X'EX} = \begin{bmatrix} SS_{X_1} & SP_{X_1X_2} & \cdots & SP_{X_1X_p} \\ SP_{X_2X_1} & SS_{X_2} & \cdots & SP_{X_2X_p} \\ \vdots & \vdots & \ddots & \vdots \\ SP_{X_pX_1} & SP_{X_pX_2} & \cdots & SS_{X_p} \end{bmatrix}$$

4.5 (Co)variance

4.5.1 Variance

Recall that the sample variance is:

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

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

$$s_X^2 = \frac{1}{n-1} \Big(\textbf{X}' \; \textbf{X} - \frac{1}{n} \; \big(\textbf{X}' \; \textbf{E} \; \textbf{X} \big) \Big)$$

4.5.2 Covariance

Recall that the *sample covariance* is:

$$cov_{XY} = s_{XY} = \frac{covariation}{n-1} = \frac{SP_{XY}}{n-1}$$

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

$$cov_{XY} = s_{XY} = \frac{1}{n-1} \Big(\mathbf{X}' \; \mathbf{Y} - \frac{1}{n} \; \big(\mathbf{X}' \; \mathbf{E} \; \mathbf{Y} \big) \Big)$$

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

$$\mathbf{S}_{XX} = \frac{1}{n-1}(\mathbf{X'X} - \frac{1}{n}\mathbf{X'EX}) = \begin{bmatrix} s_{X_1}^2 & s_{X_1X_2} & \cdots & s_{X_1X_p} \\ s_{X_2X_1} & s_{X_2}^2 & \cdots & s_{X_2X_p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{X_pX_1} & s_{X_pX_2} & \cdots & s_{X_p}^2 \end{bmatrix}$$

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 $\mathbf{variation}$ 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 (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 (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:

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