2023 Winter School

Introduction to matrix algebra

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Matrix Algebra

- Why?
  - Store many numbers using a single symbol
  - Compact
  - Many known results written in matrix form

Introduction to Matrix Algebra: Outline

- Why matrix algebra is important

- Definition of a matrix & some special types of matrices
- Matrix operations; multiplication by scalar, addition/subtraction, multiplication, inverse, transpose

- Intro to PCA - Principal Component Analysis railway car

What is a matrix?

A rectangular array of numbers set in <u>rows</u> and <u>columns</u>,

e.g. **B** is a 2x3 matrix

$$\boldsymbol{B} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix}$$

OR

$$\boldsymbol{B} = \begin{bmatrix} 4 & 1 & 3 \\ 5 & -1 & 2 \end{bmatrix}$$

b_{ij} is the *ij* element of the matrix

Vector is a matrix with either 1 row or 1 column, e.g.

$\boldsymbol{w} = \begin{bmatrix} 7 \\ 1 \end{bmatrix}$ is a 2x1 column vector

OR

$\boldsymbol{v} = \begin{bmatrix} 3 & 5 \end{bmatrix}$ is a 1x2 row vector

Special types of matrices

- Square matrix

  (equal number of rows & columns)

$$\boldsymbol{G} = \begin{bmatrix} 1 & 3 & 7 \\ 9 & 4 & 3 \\ 2 & 1 & 2 \end{bmatrix}$$

off-diagonal elements

diagonal elements

- Diagonal matrix

  (sq. matrix with 0's for all off-diagonal elements)

$$\boldsymbol{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

- Identity matrix

  (diagonal matrix with 1's for all diagonal elements)

$$\boldsymbol{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Special types of matrices

- 'J' matrix

A vector of 1's, written **1** (or sometimes $\mathbf{1_n}$)

- Symmetric matrix

A square matrix where element *ij* equals element *ji*, e.g.

$$\boldsymbol{A} = \begin{bmatrix} 1 & 3 & 7 \\ 3 & 4 & -3 \\ 7 & -3 & 2 \end{bmatrix}$$

i.e.,
$a_{12} = a_{21} = 3$
$a_{13} = a_{31} = 7$
$a_{23} = a_{32} = -3$

Special types of matrices, partitioned matrices

- A matrix that has been broken into sections or ‘blocks’
- For convince / shorthand

e.g.

$$E = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

where:

- A is a n x 1 matrix
- B is a n x p matrix
- C is a q x 1 matrix
- D is a q x p matrix

...and E is therefore a (n+q) x (1+p) matrix

Matrix operations: multiplication by scalar

- A ‘scalar’ is a 1x1 matrix, or an ordinary number
- multiply each element of matrix by the scalar

$$\boldsymbol{2B} = 2\begin{bmatrix} 4 & 1 & 3 \\ 5 & -1 & 2 \end{bmatrix}$$

$$= \begin{bmatrix} 4x2 & 1x2 & 3x2 \\ 5x2 & -1x2 & 2x2 \end{bmatrix}$$

$$= \begin{bmatrix} 8 & 2 & 6 \\ 10 & -2 & 4 \end{bmatrix}$$

Matrix operations: Addition or subtraction

- Only possible if matrices have same number of rows and columns

(i.e. they are of the same <u>order</u> and are 'conformable')

Let $\boldsymbol{W} = \boldsymbol{X} + \boldsymbol{Y}$,

with $\boldsymbol{X}$ and $\boldsymbol{Y}$ being 2x2 matrices of $\boldsymbol{X} = \begin{bmatrix} \mathbf{3} & \mathbf{5} \\ \mathbf{-1} & \mathbf{2} \end{bmatrix}$ and $\boldsymbol{Y} = \begin{bmatrix} \mathbf{1} & \mathbf{7} \\ \mathbf{2} & \mathbf{9} \end{bmatrix}$

$$\boldsymbol{W} = \boldsymbol{X} + \boldsymbol{Y} = \begin{bmatrix} \boldsymbol{x}_{\mathbf{11}} + \boldsymbol{y}_{\mathbf{11}} & \boldsymbol{x}_{\mathbf{12}} + \boldsymbol{y}_{\mathbf{12}} \\ \boldsymbol{x}_{\mathbf{21}} + \boldsymbol{y}_{\mathbf{21}} & \boldsymbol{x}_{\mathbf{22}} + \boldsymbol{y}_{\mathbf{22}} \end{bmatrix}$$

$$\boldsymbol{W} = \begin{bmatrix} \mathbf{3+1} & \mathbf{5+7} \\ \mathbf{-1+2} & \mathbf{2+9} \end{bmatrix} = \begin{bmatrix} \mathbf{4} & \mathbf{9} \\ \mathbf{1} & \mathbf{11} \end{bmatrix}$$

Matrix operations: Transpose

- The transpose of matrix $\boldsymbol{B}$ is usually written $\boldsymbol{B}'$ (or sometimes $\boldsymbol{B}^{\boldsymbol{T}}$)
- The transpose of $\boldsymbol{B}$ is the matrix whose element *ji* are equal to the *ij* element of $\boldsymbol{B}$ i.e. $b_{ij} = b'_{ji}$
  - ➢Turn the columns of $\boldsymbol{B}$ into the rows of $\boldsymbol{B}'$

If $\boldsymbol{B} = \begin{bmatrix} 4 & 1 & 3 \\ 5 & -1 & 2 \end{bmatrix}$ then $\boldsymbol{B}' = \begin{bmatrix} 4 & 5 \\ 1 & -1 \\ 3 & 2 \end{bmatrix}$

Note that $\boldsymbol{B} \neq \boldsymbol{B}'$ (unless $\boldsymbol{B}$ is symmetric)

Matrix operations: multiplication

- Order is important!
- Only possible if number of columns 1st matrix = number of rows 2nd matrix

If $\mathbf{A}$ has order r *x* c & $\mathbf{B}$ has order c *x* n

- then $\mathbf{AB}$ exists with order r *x* n
- The ij element of $\mathbf{AB}$ is 'sum product' of row i from matrix $\mathbf{A}$ and column j from $\boldsymbol{B}$

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 0 & 5 \end{bmatrix}, B = \begin{bmatrix} 2 & 3 \\ 1 & 4 \end{bmatrix}$$

$$AB = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \\ a_{31}b_{11} + a_{32}b_{21} & a_{31}b_{12} + a_{32}b_{22} \end{bmatrix} = \begin{bmatrix} 1x2 + 2x1 & 1x3 + 2x4 \\ 2x2 + 3x1 & 2x3 + 3x4 \\ 0x2 + 5x1 & 0x3 + 5x4 \end{bmatrix} = \begin{bmatrix} 4 & 11 \\ 7 & 18 \\ 5 & 20 \end{bmatrix}$$

Matrix operations: multiplication

- Order is important!
- If $\mathbf{A}$ has order r *x* c & $\mathbf{B}$ has order c *x* n
- then $\mathbf{AB}$ exists with order r *x* n
  - $\mathbf{BA}$ doesn't exist unless r = n
  - Even if $\mathbf{BA}$ exists it isn't necessarily equal to $\mathbf{AB}$

- e.g. if $\mathbf{A}$ is a 3x2 and $\boldsymbol{B}$ is a 2x3 then
  - $\mathbf{AB}$ is a 3x3 matrix
  - $\mathbf{BA}$ is a 2x2 matrix

Matrix operations: multiplication

- Why define it this way?
- It's useful

e.g. to store simultaneous equations

2x + 3y = 15

x - y = 1

can be rewritten as $\mathbf{Av} = \mathbf{b}$; where $\mathbf{A} = \begin{bmatrix} \mathbf{2} & \mathbf{3} \\ \mathbf{1} & \mathbf{-1} \end{bmatrix}$, $\mathbf{v} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}$ & $\mathbf{b} = \begin{bmatrix} \mathbf{15} \\ \mathbf{1} \end{bmatrix}$

Matrix operations: multiplication

- The identity matrix (matrix with 1's on diagonal) has a special property,
  - ➢Any matrix multiplied by its identity matrix returns the original matrix

- If $\mathbf{A} = \begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix}$, the $\mathbf{AI} = \mathbf{A}$

Let's try it: $\begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2x1 + 3x0 & 2x0 + 3x1 \\ 1x1 - 1x0 & 1x0 - 1x1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix}$

Matrix operations: inverse

- Some (not all!) square matrices have an inverse
- The inverse of $\mathbf{A}$ is written as $\boldsymbol{A}^{-\mathbf{1}}$
- The inverse of a matrix is one where when multiplied by the original matrix, it returns the identity matrix
    - $\mathbf{A}^{-\mathbf{1}}\mathbf{A} = \mathbf{I}$
- Relatively easy to calculate for 2x2 matrix:
    - If $\mathbf{A} = \begin{bmatrix} \boldsymbol{a}_{11} & \boldsymbol{a}_{12} \\ \boldsymbol{a}_{21} & \boldsymbol{a}_{22} \end{bmatrix}$ then
    - $\boldsymbol{A}^{-1} = \frac{\mathbf{1}}{|\boldsymbol{A}|}\begin{bmatrix} \boldsymbol{a}_{22} & -\boldsymbol{a}_{12} \\ -\boldsymbol{a}_{21} & \boldsymbol{a}_{11} \end{bmatrix}$ where |A| is the determinate of A, and
    - |A| = $(\boldsymbol{a}_{11}\boldsymbol{a}_{22} - \boldsymbol{a}_{12}\boldsymbol{a}_{21})$

Matrix operations: calculating the inverse

$$\mathbf{A} = \begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix}$$

$$A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$

$$= \frac{1}{(-5)} \begin{bmatrix} -1 & -3 \\ -1 & 2 \end{bmatrix}$$

$$= \begin{bmatrix} 1/5 & 3/5 \\ 1/5 & -2/5 \end{bmatrix}$$

Sanity check: $\mathbf{A}^{-1}\mathbf{A} = \begin{bmatrix} 1/5 & 3/5 \\ 1/5 & -2/5 \end{bmatrix} \begin{bmatrix} 2 & 3 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} \frac{2}{5} + \frac{3}{5} & \frac{3}{5} - \frac{3}{5} \\ \frac{2}{5} - \frac{2}{5} & \frac{3}{5} + \frac{2}{5} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Note: calculating the inverse is usually done by computer programs

A unique inverse cannot be calculated if the determinate is zero,
[1] the matrix is said to be singular
[2] need to use a generalized inverse

Matrix operations: example

We have measured the weight of 6 people, what is their mean weight?

Let $\boldsymbol{w}$ be the 1x6 row vector of weights

$\mathbf{1}'\boldsymbol{w}$ gives the sum of the elements of $\boldsymbol{w}$

$\mathbf{1}'\boldsymbol{w}/\boldsymbol{n}$ is the average of the elements of $\boldsymbol{w}$

$$\boldsymbol{w} = [53 \quad 60 \quad 85 \quad 70 \quad 72 \quad 64]$$

$$\mathbf{1}'\boldsymbol{w} = 404$$

$$\mathbf{1}'\boldsymbol{w}/\mathbf{6} = 67.3$$

Matrix operations: example

e.g. simultaneous equations

2x + 3y = 15

 x - y = 1

can be rewritten as $\mathbf{Av} = \mathbf{b}$; where $\mathbf{A} = \begin{bmatrix} \mathbf{2} & \mathbf{3} \\ \mathbf{1} & \mathbf{-1} \end{bmatrix}$, $\mathbf{v} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}$& $\mathbf{b} = \begin{bmatrix} \mathbf{15} \\ \mathbf{1} \end{bmatrix}$

What values are x and y?

$$\mathbf{Av} = \mathbf{b}$$
$$\boldsymbol{A}^{-\mathbf{1}}\mathbf{Av} = \boldsymbol{A}^{-\mathbf{1}}\mathbf{b}$$
$$\mathbf{v} = \boldsymbol{A}^{-\mathbf{1}}\mathbf{b}$$

$$= \begin{bmatrix} \mathbf{0.2} & \mathbf{0.6} \\ \mathbf{0.2} & \mathbf{-0.4} \end{bmatrix} \begin{bmatrix} \mathbf{15} \\ \mathbf{1} \end{bmatrix} = \begin{bmatrix} \mathbf{0.2}\boldsymbol{x}\mathbf{15} + \mathbf{0.6}\boldsymbol{x}\mathbf{1} \\ \mathbf{0.2}\boldsymbol{x}\mathbf{15} - \mathbf{0.4}\boldsymbol{x}\mathbf{1} \end{bmatrix} = \begin{bmatrix} \mathbf{3.6} \\ \mathbf{2.6} \end{bmatrix}$$

PCA analysis

- PCA (Principal component analysis) is a useful method to summarize the ‘essence’ of your data
  - ➢ Dimension reduction technique
- Based on *eigen-decomposition* of a diagonalizable matrix
- Exact methods (R/GCTA/EIGENSTRAT) are computationally expensive for large datasets
  - Approximate methods, e.g. fastPCA

- Good 20min step-by-step intro PCA analysis on YouTube, StatQuest
  - ➢ https://www.youtube.com/watch?v=FgakZw6K1QQ

Example: PCA analysis in UK Biobank

- Bycroft et al 2018 Nature
- Genomic relationship matrix is a n x n matrix of SNP relationships between individuals
- Software: fastPCA
  - also possible in GCTA for smaller datasets

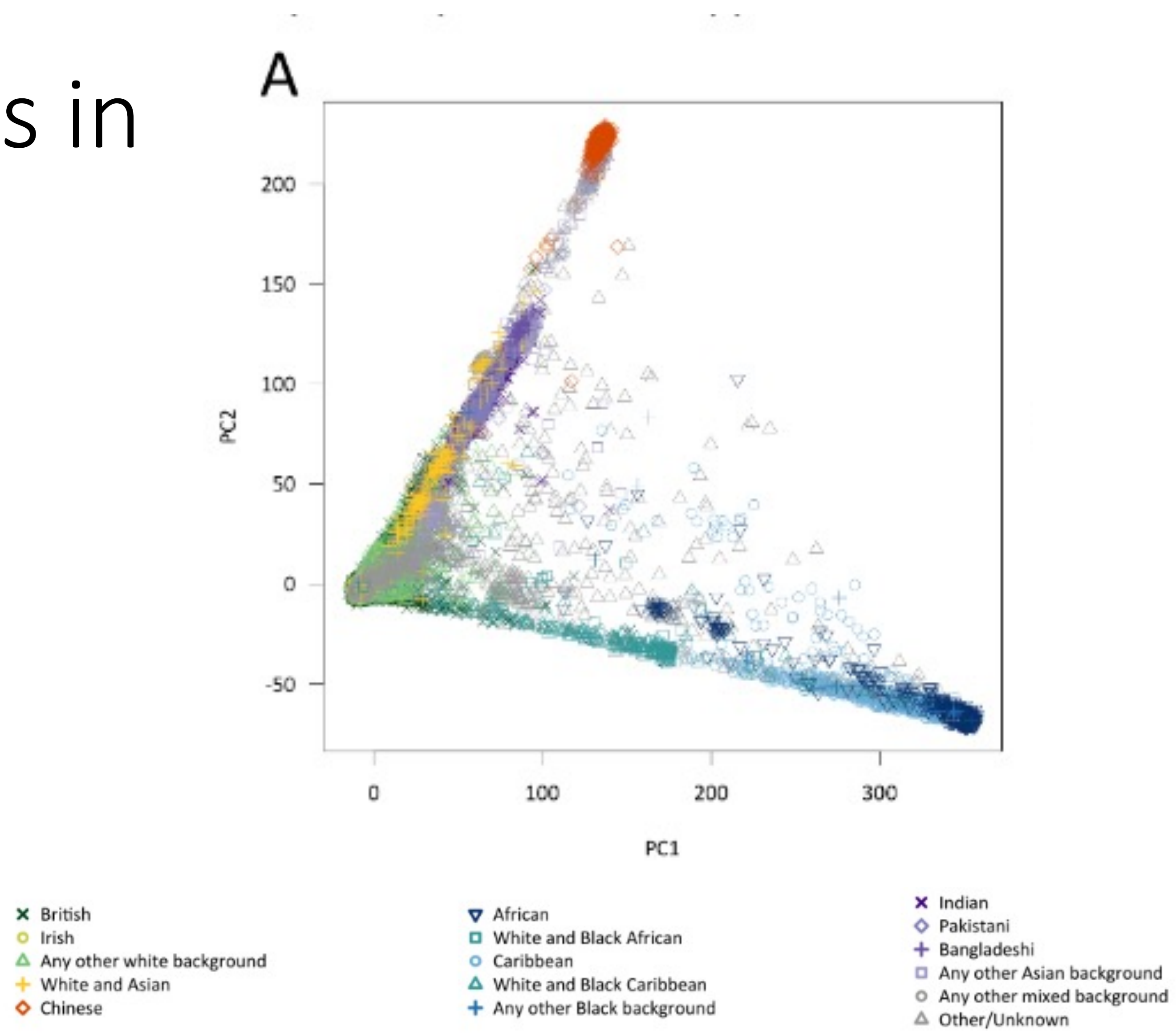

Figure 2 Genetic principal components in UK Biobank, computed from 141,0670 samples and 101,284 SNPs using flashPCA [10]. **(A)** The 1st principal component (PC1) on the *x*-axis and the 2nd principal component (PC2) on the *y*-axis. **(B)** The 3rd principal component (PC3) on the *x*-axis and the 4th principal component (PC4) on the *y*-axis. In both panels, samples are coloured according to self-reported ethnicity. The legend indicates the coloured symbol used for each predefined ethnicity throughout this document.

A brief introduction to: Eigenvalues and eigenvectors

- Given a square matrix **A**,
  - Can we define a vector **v** and scalar **b** such that **Av** = b**v**? If so then b is an eigenvalue and **v** an eigenvector of **A**.
  - Note:
    - Eigen values and eigen vectors work as a 'pair'
    - there maybe 0 to n (where n is the rank of **A**) eigenvalue/eigenvector pairs for **A**
    - e.g.

Is $\mathbf{v}$= $\begin{bmatrix} \mathbf{2} \\ \mathbf{1} \end{bmatrix}$ and b =4 an eigenvector/eigenvalue pair of $\mathbf{A}$ = $\begin{bmatrix} \mathbf{3} & \mathbf{2} \\ \mathbf{3} & \mathbf{-2} \end{bmatrix}$?

b**v = 4** $\begin{bmatrix} \mathbf{2} \\ \mathbf{1} \end{bmatrix}$= $\begin{bmatrix} \mathbf{8} \\ \mathbf{4} \end{bmatrix}$

Av= $\begin{bmatrix} \mathbf{3} & \mathbf{2} \\ \mathbf{3} & \mathbf{-2} \end{bmatrix} \begin{bmatrix} \mathbf{2} \\ \mathbf{1} \end{bmatrix}$

= $\begin{bmatrix} \mathbf{3x2 + 2x1} \\ \mathbf{3x2 - 2x1} \end{bmatrix}$= $\begin{bmatrix} \mathbf{8} \\ \mathbf{4} \end{bmatrix}$

Eigenvalues, eigenvectors & PCA analysis

- In PCA,
  - Eigenvalues are ordered, largest to smallest
  - Eigenvectors are orthogonal
- PC1 (1^{st} principal component) has the largest eigenvalue. PC1 represents the largest axis of variation in the matrix.
- PC2 is orthogonal (uncorrelated) to PC1 and has the 2nd largest eigenvalue. It represents the 2^{nd} largest axis of variation in the matrix.
  - ...etc.
- e.g. $\mathbf{K}$ is decomposed into eigenvalues $\mathbf{D}$ and eigenvectors $\mathbf{E}$, then $\mathbf{K} = \mathbf{EDE}'$

Eigenvalues, eigenvectors & PCA analysis

What is the primary axis of variation in $\mathbf{K}$, if $\boldsymbol{K} = \begin{bmatrix} 1348 & 66.5 & -117.7 \\ 66.5 & 24.3 & -14.0 \\ -111.7 & -14.0 & 14.5 \end{bmatrix}$

Let $\mathbf{K} = \mathbf{EDE}'$

where **D** is the eigenvalues, $\boldsymbol{D} = \begin{bmatrix} 1361 & 0 & 0 \\ 0 & 24.5 & 0 \\ 0 & 0 & 1.5 \end{bmatrix}$

and **E** are the eigenvectors, $\boldsymbol{E} = \begin{bmatrix} -0.995 & -0.079 & 0.056 \\ -0.050 & 0.915 & 0.400 \\ 0.083 & -0.395 & 0.915 \end{bmatrix}$

basics – practical 1

- Some matrix algebra to do by-hand (!)

- Work through “basicsPrac1.pdf”
    - PART 1: check answers to matrix algebra questions
    - PART 2: Small example PCA analysis

- Software: R

Cluster Access

- You have all been provided with login details to computing resources needed for the practical component

- An SSH terminal is needed to connect to the computing:
  - Windows: Install PuTTY
  - Hostname: as provided (203.101.228.xxx)
  - User: as provided
  - Check Connection > SSH > X11 > Enable X11 forwarding

  - Mac/Linux: Use the terminal
  - `ssh -X <user>@203.101.228.xxx`