Scientific Computing for Biologists

Introduction to matrices

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Introduction to Matrices

- One way to think about a matrix is as a collection of vectors. This is, in essence, what a multivariate data set is.
- A matrix which has n rows and p columns will be referred to as a $n \times p$ matrix. $n \times p$ is the shape of the matrix.

$$\underset{(n\times p)}{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix}$$

Special Matrices

- Zero matrix

$$\mathbf{0} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

- Square matrix
  A matrix whose shape is is $n \times n$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

- Ones matrix

$$\mathbf{1} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

- Diagonal matrix
  A square matrix where the off-diagonal elements are zero.

$$A = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}$$

Scalar Multiplication of a Matrix

- Let k be a scalar and let A be the matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix}$$

- then

$$kA = \begin{bmatrix} ka_{11} & ka_{12} & \cdots & ka_{1p} \\ ka_{21} & ka_{22} & \cdots & ka_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ ka_{n1} & ka_{n2} & \cdots & ka_{np} \end{bmatrix}$$

Addition and Subtraction of Matrices

- Let A and B be matrices that have the same shape, $n \times p$:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix} \quad B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1p} \\ b_{21} & b_{22} & \cdots & b_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{np} \end{bmatrix}$$

- then

$$A + B = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \cdots & a_{1p} + b_{1p} \\ a_{21} + b_{11} & a_{22} + b_{22} & \cdots & a_{2p} + b_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} + b_{n1} & a_{n2} + b_{n2} & \cdots & a_{np} + b_{np} \end{bmatrix}$$

$$A - B = A + (-B)$$

Multiplying a Matrix by a Vector

- Let A be a $n \times p$ matrix, and let $\boldsymbol{x}$ be a $p \times 1$ column vector

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix}$$

- then

$$A\boldsymbol{x} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1p}x_p \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2p}x_p \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{np}x_p \end{bmatrix}$$

Note that $A\boldsymbol{x}$ is a vector with shape $n \times 1$. The i-the element of $A\boldsymbol{x}$ is equivalent to the dot product of the i-th row vector of A with $\boldsymbol{x}$.

Matrices as Linear Transformations

- Let A be a particular $n \times p$ matrix. Than for any p-vector $\boldsymbol{x}$, the product $A\boldsymbol{x}$ is a n-vector.
- We say that the matrix A determines a function from $\mathbb{R}^p$ to $\mathbb{R}^n$.
  - $A(k\boldsymbol{x}) = k(A\boldsymbol{x})$ where k is a scalar.
  - If $\boldsymbol{y}$ is also a p-vector than $A(\boldsymbol{x} + \boldsymbol{y}) = A\boldsymbol{x} + A\boldsymbol{y}$ is an n-vector
- A function, f, where $f(\boldsymbol{x} + \boldsymbol{y}) = f(\boldsymbol{x}) + f(\boldsymbol{y})$ and $f(k\boldsymbol{x}) = kf(\boldsymbol{x})$ is called a ***linear transformation***.

Highlight

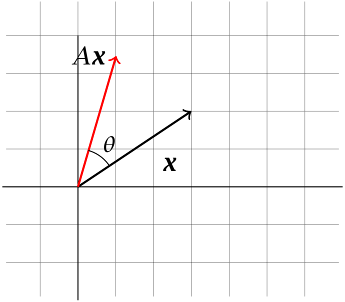
Every matrix determines a linear transformation!

Every linear transformation can be represented by a matrix!

Examples of Linear Transformation: Rotation

- The rotation of the plane, by an angle θ about the origin is given by:

$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$



Examples of Linear Transformation in $\mathbb{R}^2$

What matrices represent these transformation in the Cartesian plane ($\mathbb{R}^2$)?

- reflection in the x-axis

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} x \\ -y \end{bmatrix}$$

- reflection in the line $y = x$

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} y \\ x \end{bmatrix}$$

- shear parallel to the x-axis

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} x + ay \\ y \end{bmatrix}$$

- projection onto the x-axis

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} x \\ 0 \end{bmatrix}$$

- How about reflection in the y-axis? shear parallel to the y-axis? projection onto the y-axis?

General Matrix Multiplication

- Let A be a $n \times p$ matrix and B be a $p \times q$ matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix} \quad B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1q} \\ b_{21} & b_{22} & \cdots & b_{2q} \\ \vdots & \vdots & \vdots & \vdots \\ b_{p1} & b_{n2} & \cdots & b_{nq} \end{bmatrix}$$

- The product AB is an $n \times q$ matrix whose (i, j)-entry is the dot product of the i-th row vector of A and the j-th column vector of B.
- A and B muse be *conformable* to calculate the product AB, i.e. the number of columns in A must be the same as the number of rows in B.

Matrix Arithmetic Rules

i. $A + B = B + A$
ii. $(A + B) + C = A + (B + C)$
iii. $k(A + B) = kA + kB$
iv. $(kA)B = k(AB)$
v. $(AB)C = A(BC)$ (associative)
vi. $A(B + C) = AB + AC$ (distributive)
vii. $(A + B)C = AC + BC$ (distributive)

Alert

Matrix multiplication is ***not*** *commutative, i.e.* $AB \neq BA$ *in general.*

Be careful when you expand expressions like $(A + B)(A + B)$.

Matrix Transpose

- We denote the transpose of a matrix as A^T
- If A is an $n \times p$ matrix, then A^T is a $p \times n$ matrix where $A^T_{ji} = A_{ij}$
- Transpose rules:
  - $(A^T)^T = A$
  - $(A + B)^T = A^T + B^T$
  - $(AB)^T = B^T A^T$
- Symmetric matrix– square matrix, A, where $A^T = A$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix}$$

$$A^T = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \vdots & \vdots \\ a_{1p} & a_{12} & \cdots & a_{np} \end{bmatrix}$$

Identity matrix

An *identity matrix* is a $p \times p$ matrix with ones on the diagonal and zeros everywhere else.

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

- $IA = AI = A$ if I and A are $n \times p$ matrices
- $A = I\boldsymbol{x}$ is a diagonal matrix where $a_{ii} = x_i$ if I is an $n \times n$ matrix and $\boldsymbol{x}$ is a $n \times 1$ vector.

Matrix Inverse

- If A is a *square matrix* and C is a matrix of the same size where $AC = I$ and $CA = I$ than C is the inverse of A and we denote it as A^{-1}.
$$AA^{-1} = A^{-1}A = I$$
- Rules for inverses:
  - Only square matrices are invertible; but not every square matrix can be inverted
  - A matrix for which we can find an inverse is called ***invertible*** (non-singular)
  - A matrix for which no inverse exists is ***singular*** (non-invertible)
  - Any diagonal matrix, A, where the a_{ii} are non-zero, is invertible
  - If A and B are both invertible $p \times p$ matrices than $(AB)^{-1} = B^{-1}A^{-1}$ (note change in order).

Descriptive statistics as matrix functions

Mean vector and mean matrix

Assume you have a data set represented as a $n \times p$ matrix, $\boldsymbol{X}$, with observations in rows and variables in columns.

Mean vector

To calculate a row vector of means, $\boldsymbol{m} = [\overline{X}_1, \overline{X}_2, \ldots, \overline{X}_p]$

$$\boldsymbol{m} = \frac{1}{n} \mathbb{1}^T \boldsymbol{X}$$

where $\mathbb{1}$ is a $n \times 1$ column vector of ones.

Matrix of column means

$$\boldsymbol{M} = \mathbb{1} \boldsymbol{m}$$

Deviation matrix

To re-express each value as the deviation from the variable means (i.e. each column is a mean centered vector) we calculate a deviation matrix:

$$\boldsymbol{D} = \boldsymbol{X} - \boldsymbol{M}$$

Covariance and correlation matrices

Covariance matrix

$$\boldsymbol{S} = \frac{1}{n-1}\boldsymbol{D}^T\boldsymbol{D}$$

Correlation matrix

$$\boldsymbol{R} = \boldsymbol{V}\boldsymbol{S}\boldsymbol{V}$$

where $\boldsymbol{V}$ is a $p \times p$ diagonal matrix where $\boldsymbol{V}_{ii} = 1/\sqrt{\boldsymbol{S}_{ii}}$.

Simultaneous Linear Equations

Simultaneous Linear Equations

- A set of simultaneous linear equations are equations like the following:

$$
\begin{aligned}
2x + y &= 4 \\
x - y &= -1
\end{aligned}
$$

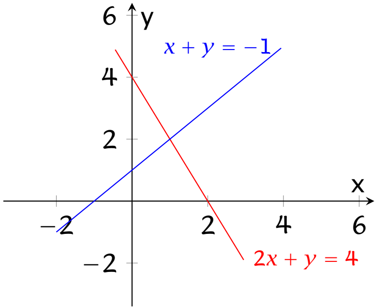
or

$$
\begin{aligned}
x + 3y + 2z &= 3 \\
-x + y + 2z &= -2 \\
2x + 4y - 2z &= 10
\end{aligned}
$$

Solving Simultaneous Linear Equations

Solving a set of simultaneous equations means to find values of the variables where all the equations are true.

$$\begin{aligned} 2x + y &= 4 \\ x - y &= -1 \end{aligned}$$



Solutions to Simultaneous Linear Equations

Solutions to simultaneous linear equations have either:

- No solutions – inconsistent
- One solution – consistent
- Infinitely many solutions – underdetermined

Matrices and Simultaneous Linear Equations

- Matrices can be used to represent and solve simultaneous linear equations. For example,

$$\begin{aligned} x_1 + 3x_2 + 2x_3 &= 3 \\ -x_1 + x_2 + 2x_3 &= -2 \\ 2x_1 + 4x_2 - 2x_3 &= 10 \end{aligned}$$

  Can be represented by the equation $A\boldsymbol{x} = \boldsymbol{h}$:

$$\begin{bmatrix} 1 & 3 & 2 \\ -1 & 1 & 2 \\ 2 & 4 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -2 \\ 10 \end{bmatrix}$$

- Solve this equation by pre-multiplying both sides of the equation by A^{-1}.

$$\begin{aligned} A^{-1}A\boldsymbol{x} &= A^{-1}\boldsymbol{h} \\ \boldsymbol{x} &= A^{-1}\boldsymbol{h} \end{aligned}$$

Simultaneous Equations and Matrix Inverses

- $A\boldsymbol{x} = \boldsymbol{h}$ has a unique solution iff A is invertible.
- If A is a singular matrix than $A\boldsymbol{x} = \boldsymbol{h}$ either has no solution or infinitely many solutions.

Matrix Concepts

Space Spanned by a List of Vectors

Definition

Let X be a finite list of n-vectors. The **space spanned** by X is the set of all vectors that can be written as linear combinations of the vectors in X.

Remember that a *linear combination* of vectors is an equation of the form $z = b_1\boldsymbol{x}_1 + b_2\boldsymbol{x}_2 + \cdots + b_p\boldsymbol{x}_p$

Linear dependence and independence

- A list of vectors, $\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_p$, is said the be ***linearly dependent*** if there is a non-trivial linear combination of them which is equal to the zero vector.

$$b_1\boldsymbol{x}_1 + b_2\boldsymbol{x}_2 + \cdots + b_p\boldsymbol{x}_p = 0$$

- A list of vectors that are not linearly dependent are said to be ***linearly independent***

Subspaces

$\mathbb{R}^n$ denotes the seat of real n-vectors - the set of all $n \times 1$ matrices with entries from the set $\mathbb{R}$ of real numbers.

Definition

A **subspace** of $\mathbb{R}^n$ is a subset S of $\mathbb{R}^n$ with the following properties:

1. $0 \in S$
2. If $\boldsymbol{u} \in S$ then $k\boldsymbol{u} \in S$ for all real numbers k
3. If $\boldsymbol{u} \in S$ and $\boldsymbol{v} \in S$ then $\boldsymbol{u} + \boldsymbol{v} \in S$

Examples of subspaces of $\mathbb{R}^2$:

- The zero vector $\begin{bmatrix} 0 & 0 \end{bmatrix}^T$
- The zero vector plus any line in $\mathbb{R}^2$
- All of $\mathbb{R}^2$ (i.e. the entire Cartesian plane)

Basis

Let S be a subspace of $\mathbb{R}^n$. Then there is a finite list, X, of vectors from S such that S is the space spanned by X.

Let S be a subspace of $\mathbb{R}^n$ spanned by the list $(u_1, u_2, \ldots, u_n)$. Then there is a linearly independent sublist of $(u_1, u_2, \ldots, u_n)$ that also spans S.

Definition

A list X is a **basis** for S if:

- X is linearly independent
- S is the subspace spanned by X

Dimension

Let S be a subspace of $\mathbb{R}^n$.

Definition

The **dimension** of S is the number of elements in a basis for S.

Rank of a Matrix

Let A by an $n \times p$ matrix.

Definition

The **rank** of A is equal to the dimension of the row or column space of A.

Where the row space of A is the space spanned by the row vectors of A and the column space of A is defined similarly.