

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.

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

Special Matrices

■ Zero matrix

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

■ Square matrix

A matrix whose shape is $n \times n$

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

■ Ones matrix

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

■ Diagonal matrix

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

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

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 \mathbf{x} be a $p \times 1$ column vector

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

- then

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

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

Matrices as Linear Transformations

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

Highlight

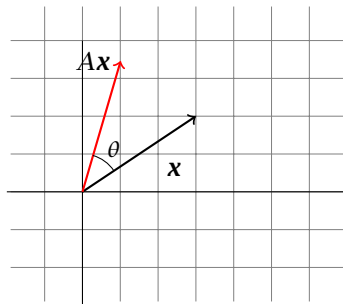
Every matrix determines a linear transformation!

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:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix} \quad B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1q} \\ b_{21} & b_{22} & \cdots & b_{2q} \\ \vdots & \vdots & \vdots & \vdots \\ b_{p1} & b_{p2} & \cdots & b_{pq} \end{bmatrix}$$

- 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 must 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 $A_{ji}^T = A_{ij}$
- 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 $A^T = A$

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

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

Identity matrix

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

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

- $IA = AI = A$ if I and A are $n \times p$ matrices
- $A = I\mathbf{x}$ is a diagonal matrix where $a_{ii} = x_i$ if I is an $n \times n$ matrix and \mathbf{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 $CA = I$ then 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 then $(AB)^{-1} = B^{-1}A^{-1}$ (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, X , with observations in rows and variables in columns.

Mean vector

To calculate a row vector of means, $\mathbf{m} = [\bar{X}_1, \bar{X}_2, \dots, \bar{X}_p]$

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

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

Matrix of column means

$$M = \mathbf{1} \mathbf{m}$$

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:

$$D = X - M$$

Covariance and correlation matrices

Covariance matrix

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

Correlation matrix

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

where \mathbf{V} is a $p \times p$ diagonal matrix where $V_{ii} = 1/\sqrt{S_{ii}}$.

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

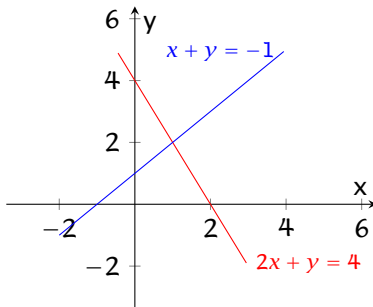
$$\begin{aligned}x + 3y + 2z &= 3 \\ -x + y + 2z &= -2 \\ 2x + 4y - 2z &= 10\end{aligned}$$

Solving Simultaneous Linear Equations

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

$$2x + y = 4$$

$$x - y = -1$$



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 $A\mathbf{x} = \mathbf{h}$:

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

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

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

Simultaneous Equations and Matrix Inverses

- $A\mathbf{x} = \mathbf{h}$ has a unique solution iff A is invertible.
- If A is a singular matrix then $A\mathbf{x} = \mathbf{h}$ 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 $z = b_1\mathbf{x}_1 + b_2\mathbf{x}_2 + \cdots + b_p\mathbf{x}_p$

Linear dependence and independence

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

$$b_1\mathbf{x}_1 + b_2\mathbf{x}_2 + \dots + b_p\mathbf{x}_p = \mathbf{0}$$

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

Subspaces

\mathbb{R}^n denotes the set 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 $\mathbf{u} \in S$ then $k\mathbf{u} \in S$ for all real numbers k
- 3 If $\mathbf{u} \in S$ and $\mathbf{v} \in S$ then $\mathbf{u} + \mathbf{v} \in S$

Examples of subspaces of \mathbb{R}^n :

- any space spanned by a list of vectors in \mathbb{R}^n
- the set of all solutions to an equation $A\mathbf{x} = 0$ where A is a $p \times n$ matrix, for any number p .

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, \dots, u_n) . Then there is a linearly independent sublist of (u_1, u_2, \dots, 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 be 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.