PBDB Intensive Summer Course 2007
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Review of Matrix Algebra: Definitions and Concepts

Introduction

The operations required to carry out parametric ordinations are expressed using *matrix algebra*, which provides a formal mathematical syntax for describing and manipulating matrices.

I do not expect you to master the complexities of this branch of mathematics, but I would like you to know a set of basic terms and properties in order to be prepared for the lectures on parametric ordination. My aim during lecture will be to translate these operations to geometric concepts, but you will need to be familiar with the entities in order to go through this material efficiently.

Basic Definitions

Matrix = an array of numbers with one or more rows and one or more columns:

$$X = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

x_{ij} = an element of X
i = row index (N = number of rows)
j = column index (p = number of columns)

Transpose Matrix = rows and columns of original matrix are exchanged:

$$X' = X^T = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Vector = a matrix with only one row or one column:

$$\vec{x} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \qquad \vec{x}' = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$$

column vector row vector

Scalar = a matrix with one row and one column (i.e., a regular number)

Elementary Vector Arithmetic

Vector Equality

$\vec{x} = \vec{y}$ if all their corresponding elements are equal:

$$\begin{bmatrix}1\\2\\3\end{bmatrix} = \vec{x} = \vec{y} = \begin{bmatrix}1\\2\\3\end{bmatrix}$$

Vector Addition

Add vectors by summing their corresponding elements

$$\vec{x} + \vec{y} = \vec{z} \Rightarrow \begin{bmatrix}1\\2\\3\end{bmatrix} + \begin{bmatrix}4\\5\\6\end{bmatrix} = \begin{bmatrix}5\\7\\9\end{bmatrix}$$

To be added, vectors must have the same number of elements and the same orientation. Vector subtraction works in the analogous way.

Multiplying a Vector by a Scalar

Multiply each element of the vector by the scalar:

$$2\vec{v} = 2\begin{bmatrix}1\\2\\3\end{bmatrix} = \begin{bmatrix}2\\4\\6\end{bmatrix}$$

This operation changes the length of the vector without changing its direction.

Minor Product

The sum of the products of the corresponding elements of two vectors; it is also called the *scalar*, *inner*, or *dot* product. It results in a scalar:

$$\vec{x}' \cdot \vec{y} = \begin{bmatrix}2 & 4 & 1\end{bmatrix}\begin{bmatrix}3\\1\\5\end{bmatrix} = 2\cdot 3 + 4\cdot 1 + 1\cdot 5 = 15$$

x is the "prefactor" and y is the "postfactor"; geometrically, the minor product is the *length* of the projection of one vector onto the other:

$$\vec{x}' \cdot \vec{y} = |\vec{x}||\vec{y}|\cos\theta$$

(θ is the angle formed by the two vectors if they start from the same point)
note: $\vec{v}' \cdot \vec{w} = \vec{w}' \cdot \vec{v}$ and $c\vec{v}' \cdot \vec{w} = c(\vec{v}' \cdot \vec{w})$

<u>*The minor product of a vector by itself is the sum of squares of its elements!*</u>

Major Product

This produces a matrix; it is also called the *vector*, *outer*, or *cross* product.

$$\vec{x} \times \vec{y}' = C \Rightarrow \begin{array}{cc} & \begin{bmatrix}y_1 & y_2 & y_3\end{bmatrix} \\ \begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix} & \begin{bmatrix}x_1y_1 & x_1y_2 & x_1y_3\\ x_2y_1 & x_2y_2 & x_2y_3\\ x_3y_1 & x_3y_2 & x_3y_3\end{bmatrix}\end{array} \Rightarrow \begin{array}{cc} & \begin{bmatrix}3 & 1 & 5\end{bmatrix} \\ \begin{bmatrix}2\\4\\1\end{bmatrix} & \begin{bmatrix}6 & 2 & 10\\ 12 & 4 & 20\\ 3 & 1 & 5\end{bmatrix}\end{array}$$

Special Vectors

Unit vector = $\vec{1}$ = a vector with all elements equal to 1
Zero vector = a vector with all elements equal to 0

Useful Geometric Relationships

Vector Length: $|\vec{v}| = \sqrt{\vec{v}'\cdot\vec{v}}$

Angle Between Two Vectors: $\cos\theta = \dfrac{\vec{v}'\cdot\vec{w}}{|\vec{v}||\vec{w}|} = \dfrac{\vec{v}'\cdot\vec{w}}{(\vec{v}'\cdot\vec{v})^{1/2}(\vec{w}'\cdot\vec{w})^{1/2}}$

Distance Between Two Points (i.e., Euclidean distance) = Length of the difference vector: $d = |\vec{v} - \vec{w}| = \left[(\vec{v} - \vec{w})'\cdot(\vec{v} - \vec{w})\right]^{1/2}$

Basic Matrix Arithmetic

Types of Matrices and Their Parts

N = number of rows
p = number of columns
Rectangular matrix = matrix with unequal number of rows and columns ($N \neq p$)
Square matrix = matrix with equal number of rows and columns ($N=p$)
Principal diagonal = matrix elements for which row index = column index ($i=j$)
Trace = sum of elements along principal diagonal (trA = trace of matrix A)
Symmetrical matrix = square matrix in which $a_{ij} = a_{ji}$
Diagonal matrix = a symmetrical matrix with off-diagonal elements = 0
Identity matrix = diagonal matrix with all non-zero elements = 1; indicated by the symbol I; a matrix multiplied by I equals itself (analogous to multiplication by 1 in arithmetic)
Null matrix = a matrix will all elements = 0

Two matrices are equal if all their elements are equal

Addition & Subtraction of Matrices. Add (subtract) matrices by adding (subtracting) all the corresponding elements of the matrices (the matrices must be of the same order – i.e., have the same number of rows and columns):

$$\begin{bmatrix} 1 & 3 & -2 \\ 4 & 7 & 1 \end{bmatrix} + \begin{bmatrix} 2 & -1 & 4 \\ 3 & -7 & -2 \end{bmatrix} = \begin{bmatrix} 3 & 2 & 2 \\ 7 & 0 & -1 \end{bmatrix}$$

Multiplying a Scalar by a Matrix. Multiply every element by the scalar value:

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

Multiplying Two Matrices. $C = AB$ means that every element of C is the minor product of the corresponding row vector of A and column vector of B:

$$AB = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} e & f & g \\ h & i & j \end{bmatrix} = \begin{bmatrix} ae + bh & af + bi & ag + bj \\ ce + dh & cf + di & cg + dj \end{bmatrix} = C$$

A is referred to as the "prefactor" and B is referred to as the "postfactor"; the number of columns in the prefactor must equal the number of rows in the post-factor.

Product Moment Matrices

Major Product Moment: $C = XX'$; also called the "outer product"; this produces a symmetrical matrix in which each element, c_{ij}, is the dot product of the vectors represented by row i and column j in X; $C_{i=j}$ (i.e., the principal diagonal) is the sum of squares of each row of X

Minor Product Moment: $C = X'X$; also called the "inner product"; this produces a symmetrical matrix in which each element, c_{ij}, is the dot product of the vectors represented by row j and column i in X; $C_{i=j}$ (i.e., the principal diagonal) is the sum of squares of each column of X

Results of Multiplying Matrices

Row vector · matrix = row vector:

$$\begin{bmatrix} 1 & 3 & 0 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 2 \end{bmatrix}$$

Unit row vector · matrix = row vector of sums of matrix columns:

$$\begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 3 \end{bmatrix}$$

Matrix · column vector = column vector:

$$\begin{bmatrix} 3 & 1 \\ 4 & 0 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 4 \\ 7 \end{bmatrix}$$

Matrix · unit column vector = column vector of sums of matrix rows:

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

$\vec{1}' X \vec{1}$ = *scalar that is the sum of all elements of X:*

$$\begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 9$$

Diagonal matrix · X = matrix whose elements in ith *row equal the elements in* ith *row of X multiplied by* ith *element of diagonal matrix:*

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 4 \\ 3 & 0 \\ 2 & 1 \end{bmatrix}$$

X · diagonal matrix = matrix whose elements in jth *column equal the elements in* jth *column of X multiplied by* jth *element of diagonal matrix:*

$$\begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} = \begin{bmatrix} 6 & 6 \\ 2 & 0 \\ 4 & 3 \end{bmatrix}$$

Pre- or post-multiplication by a diagonal matrix <u>*scales*</u> rows or columns of a matrix by a constant given along the principal diagonal of the diagonal matrix.

Matrix Inversion

One cannot divide one matrix by another – rather, an inverse matrix must be *multiplied* (like multiplying by the reciprocal of a number in regular arithmetic).

If C is the inverse of B, then $BC = CB = I$ (the identity matrix); this is indicated by the following notation: $C = B^{-1}$.

Not all matrices have an inverse.

Normal and Orthonormal Vectors and Matrices

Normalized vector = a vector of unit length – i.e., $(\vec{x}'\cdot\vec{x})^{1/2} = 1$; found by dividing a vector by the square root of its minor product:

$$\frac{\vec{x}}{|\vec{x}|} = \frac{\vec{x}}{(\vec{x}'\cdot\vec{x})^{1/2}}$$

Orthogonal vectors = two vectors are orthogonal (i.e., perpendicular) if their minor product equals 0 (i.e., if $\cos\theta = 0$, then $\theta = 90^\circ$)

Orthogonal matrices = a matrix is orthogonal if all possible pairs of column vectors in that matrix are orthogonal; if the minor product moment results in a diagonal matrix (i.e., the minor product of every column vector in the matrix is 0), then the matrix is orthogonal

Orthonormal matrices = a matrix is orthonormal if it is both orthogonal and all its column vectors are normalized; i.e., its minor product moment is I, the identity matrix

Factoring Matrices and Eigenanalysis

Point: understand a matrix by breaking it into constituent parts; just as numbers can be broken into factors, so can matrices; for any number or matrix, there are an infinite number of factor pairs

Rank of a matrix = the smallest possible order common to both factors of a matrix; the rank of a matrix is the smallest number of dimensions in which its constituent row and column vectors can be displayed geometrically; it equals the minimum number of linearly independent (i.e., orthogonal) vectors that are needed to serve as a frame of reference for the data in the matrix.

Note. The vectors in a matrix can be redundant – i.e., they can be multiples or combinations of each other

Eigenanalysis finds the factors of a matrix with certain particularly useful properties: a set of mutually perpendicular vectors of unit length (*eigenvectors*) and their associated *eigenvalues* (which describe the lengths of the eigenvectors); eigenvectors and eigenvalues are also called latent vectors and values, characteristic vectors and values, and proper vectors and values.

Algebra of Eigenanalysis

Start with a square, symmetrical matrix, *R* (i.e., a similarity matrix in our case)
An eigenvector of the matrix will have the following property:

$$R\vec{u} = \vec{u}\lambda$$

When *R* is multiplied by a column vector and the result is a scalar change in the vector, then the vector is an eigenvector of *R* and the scalar is the associated eigenvalue. In essence, if the row points of *R* can be projected onto the vector u without distorting their relative positions to one another (except for their absolute scale), then $\vec{u}$ is an eigenvector and λ is the corresponding eigenvalue.

This has the following implications:

$$R\vec{u} - \lambda\vec{u} = 0$$

$$(R - \lambda I)\vec{u} = 0$$

The number of non-zero eigenvectors = rank of *R* (number of orthogonal dimensions required to contain all the column vectors of *R*)

In full matrix notation:

$$RU = U\Lambda$$

$$U'U = UU' = I$$

$$R = U\Lambda U'$$

U = matrix of eigenvectors
Λ = diagonal matrix of eigenvalues
U'U = *UU'* = *I*; without proof, *U* is an orthonormal matrix – i.e., all the eigenvectors are unit length and mutually perpendicular

Point = R can be entirely factored into eigenvalues and eigenvectors!

Why is this good?

1) eigenvectors are perpendicular to one another, so they provide a coordinate system to view the column vectors of *R* (i.e., and x-y-z coordinate system)
2) $tr\Lambda = trR$ – the sum of the eigenvalues equals the sum of the elements along the principal diagonal of *R*
3) number of non-zero eigenvalues = rank of *R*