In case you don't remember all that matrix algebra off the top of your head…

Matrix Algebra and Matrix Notation:

A Brief Refresher

Scalars and Vectors

Scalar: A single value, constant, or observation.

Scalars are denoted by lowercase italics. $x = [5]$

Vector: A row or column of values, responses, or observations.

$$\text{Column vector: } \mathbf{x} = \begin{bmatrix} 5 \\ 2 \\ 4 \\ 8 \end{bmatrix}$$

Vectors are denoted by lowercase bold letters.

$$\text{Row vector: } \mathbf{x}' = \begin{bmatrix} 5 & 2 & 4 & 8 \end{bmatrix}$$

Matrices

Matrix: A rectangular array of values arranged in rows and columns, denoted by its size, *n* × *p* such that *n* is the number of rows and *p* is the number of columns.

$$2 \times 3 \text{ Matrix: } \mathbf{X} = \begin{bmatrix} 5 & 2 & 7 \\ 4 & 1 & 3 \end{bmatrix}$$

$$3 \times 2 \text{ Matrix: } \mathbf{X}' = \begin{bmatrix} 5 & 4 \\ 2 & 1 \\ 7 & 3 \end{bmatrix}$$

Matrices are denoted by uppercase bold letters.

Transpose to switch rows and columns

Special Properties of Matrices

Square: $n = p$

$$\mathbf{X}_1 = \begin{bmatrix} 2 & 3 & 6 \\ 5 & 1 & 2 \\ 5 & 8 & 0 \end{bmatrix}$$

Symmetric: Area above the diagonal is a mirror image of the area below the diagonal, or $x_{12} = x_{21}$, $x_{23} = x_{32}$,… $x_{ij} = x_{j}$.

$$\mathbf{X}_2 = \begin{bmatrix} 1 & 3 & 6 \\ 3 & 1 & 2 \\ 6 & 2 & 1 \end{bmatrix}$$

Transposing Matrices

A matrix **X** is transposed (**X'**) by changing rows to columns and columns to rows:

$$\mathbf{X} = \begin{bmatrix} 5 & 2 & 7 \\ 4 & 1 & 3 \end{bmatrix} \quad \mathbf{X}' = \begin{bmatrix} 5 & 4 \\ 2 & 1 \\ 7 & 3 \end{bmatrix}$$

Transposing matrices can make it possible to multiply them.

Notice that for a matrix **X**, the matrix equivalent of x^2 is **X'X**.

Commonly Used Matrices

SSCP

$$\mathbf{X'X} = \begin{bmatrix} SS_1 & SP_{12} & SP_{13} \\ SP_{21} & SS_2 & SP_{23} \\ SP_{31} & SP_{32} & SS_3 \end{bmatrix}$$

Variance-covariance

$$\mathbf{S} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 \end{bmatrix}$$

Identity

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

Correlation

$$\mathbf{R} = \begin{bmatrix} 1 & r_{12} & r_{13} \\ r_{21} & 1 & r_{23} \\ r_{31} & r_{32} & 1 \end{bmatrix}$$

Summarizing Variability: Trace

Trace: Sum of diagonal elements

$$\mathbf{X}_1 = \begin{bmatrix} 2 & 3 & 6 \\ 5 & 1 & 2 \\ 5 & 8 & 0 \end{bmatrix} \qquad \mathrm{Tr}(\mathbf{X}_1) = 2 + 1 + 0 = 3$$

Summarizing Variability: Determinant

Determinant: A single value that characterizes a square matrix, the determinant represents the volume of the $n \times p$ space.

- Application: the determinant of a covariance matrix is the generalized variance of a set of variables.
- Denoted |**A**|.

Determinant: Simplest Case

The determinant of a 2 × 2 matrix is simple to calculate:

For a matrix **A**: $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$

|**A**| = *ad* - *bc*

Now consider the determinant of a 3 × 3 matrix.

Determinant of a 3 × 3 Matrix

For 3 × 3 matrices, follow the arrows:

Step 1. Add the products in one direction:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{bmatrix} \Rightarrow \begin{aligned} &(1*4*6) + (2*5*3) + (3*5*2) \\ &= 24 + 30 + 30 \\ &= 84 \end{aligned}$$

Determinant of a 3 × 3 Matrix

Step 2. Add the products in the other direction:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{bmatrix} \Rightarrow \begin{aligned} &(3*4*3) + (5*5*1) + (6*2*2) \\ &= 36 + 25 + 24 \\ &= 85 \end{aligned}$$

Determinant of a 3 × 3 Matrix

Step 3. Subtract the results of Steps 1 and 2:

$$84 - 85$$

$$|\mathbf{A}| = -1$$

Matrix Addition and Subtraction

Equal-sized matrices are added or subtracted by adding or subtracting corresponding elements:

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 10 & 8 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 6 & 12 \\ 5 & 4 \end{bmatrix}$$

$$\mathbf{A}+\mathbf{B} = \begin{bmatrix} 8 & 13 \\ 15 & 12 \end{bmatrix} \quad \mathbf{A}-\mathbf{B} = \begin{bmatrix} -4 & -11 \\ 5 & 4 \end{bmatrix}$$

Matrix Multiplication

If $p_\mathbf{A} = n_\mathbf{B}$, the sum of the products of the i^{th} row of **A** and the j^{th} column of **B** make the elements of the resulting matrix.

The resulting matrix will be of size $n_\mathbf{A} \times p_\mathbf{B}$:

$$\mathbf{AB} = \begin{bmatrix} 5 & -2 \\ 4 & 7 \\ 9 & 3 \end{bmatrix} \begin{bmatrix} -5 & 2 & 4 & 1 \\ 3 & 6 & -2 & 5 \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} 5(-5)-2(3) & 5(2)-2(6) & 5(4)-2(-2) & 5(1)-2(5) \\ 4(-5)+7(3) & 4(2)+7(6) & 4(4)+7(-2) & 4(1)+7(5) \\ 9(-5)+3(3) & 9(2)+3(6) & 9(4)+3(-2) & 9(1)+3(5) \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} -31 & -2 & 24 & -5 \\ 1 & 50 & 2 & 39 \\ -36 & 36 & 30 & 24 \end{bmatrix}$$

Matrix Division: Inverse

Inverse: The multivariate equivalent of division.

Denoted $\mathbf{A}^{-1}$

Inverse: Matrix Division

The inverse of a matrix is one that solves the following:

$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$

To find the inverse of a 2 × 2 matrix by hand, first create a pattern matrix with alternating + and – signs across each row:

$$\begin{bmatrix} + & - \\ - & + \end{bmatrix}$$

Next, find the determinant:

$$|\mathbf{A}| = \begin{vmatrix} 4 & 1 \\ 3 & 4 \end{vmatrix} = (4*4)-(1*3) = 13$$

Inverse: Matrix Division

Attach the signs from the pattern matrix to the original matrix elements and swap the elements on the positive diagonal:

$$\begin{bmatrix} 4 & -1 \\ -3 & 4 \end{bmatrix}$$

Finally, divide each element by the determinant of the matrix:

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{4}{13} & \frac{-1}{13} \\ \frac{-3}{13} & \frac{4}{13} \end{bmatrix}$$

Singular Matrices: A Real Problem

Notice that if the determinant of a matrix=0, the inverse cannot be calculated. Matrices whose determinant=0 are known as *singular* matrices.

Collinear variables in a matrix can cause singularity. Matrix inversion is used extensively in multivariate statistics, and therefore collinear variables (and singular matrices) pose a real problem for analysis.

Eigenvalues and Eigenvectors

Eigenvalue (also called a characteristic root; denoted λ):

- the consolidated variance of a square matrix
- the variance accounted for by a linear combination of the variables.

Eigenvector (also called a characteristic vector):

- a nonzero vector that forms a linear combination of a set of variables that maximizes shared variance among *p* variables.

If a matrix **A** is of size $p \times p$, then there are *p* eigenvalues of **A**. Eigenvalues can have values of less than or equal to zero.

Properties of Eigenvalues

For a square matrix **X** with *p* eigenvalues λ_i:

$$\sum_{i=1}^{p} \lambda_i = tr(\mathbf{X})$$

and

$$\prod_{i=1}^{p} \lambda_i = |\mathbf{X}|$$