

Definition: An $m \times n$ matrix, $\mathbf{A}_{m \times n}$, is a rectangular array of real numbers with m rows and n columns. Element in the i^{th} row and the j^{th} column is denoted by a_{ij} .

$$\mathbf{A}_{m \times n} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & \cdots & \cdots & a_{mn} \end{bmatrix}_{m \times n}$$

Definition: A vector \mathbf{a} of length n is an $n \times 1$ matrix with each element denoted by a_i . The i^{th} element is called the i^{th} component of the vector and n is the dimensionality.

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

Matrix Operations

- Two matrices \mathbf{A} and \mathbf{B} of the same dimensions can be added. The sum $\mathbf{A} + \mathbf{B}$ has (i, j) entry $a_{ij} + b_{ij}$. So

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \end{bmatrix}$$

$$\text{Example : } \mathbf{A} = \begin{bmatrix} 1 & 3 \\ 2 & 6 \\ -1 & -3 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 3 & 2 \\ 9 & 5 \\ 3 & 0 \end{bmatrix} \quad \mathbf{A} + \mathbf{B} = \begin{bmatrix} 4 & 5 \\ 11 & 11 \\ 2 & -3 \end{bmatrix}$$

- $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$
- $(\mathbf{A} + \mathbf{B}) + \mathbf{C} = \mathbf{A} + (\mathbf{B} + \mathbf{C})$

- A matrix may also be multiplied by a constant c . The product $c\mathbf{A}$ is the matrix that results from multiplying each element of \mathbf{A} by c . Thus

$$c\mathbf{A}_{m \times n} = \begin{bmatrix} ca_{11} & ca_{12} & \cdots & ca_{1n} \\ ca_{21} & ca_{22} & \cdots & ca_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ ca_{m1} & \cdots & \cdots & ca_{mn} \end{bmatrix}_{m \times n}$$

3. The **transpose** operation \mathbf{A}^T or \mathbf{A}' of a matrix changes the columns into rows so that the first column of \mathbf{A} becomes the first row of \mathbf{A}^T , the second column becomes second row, and etc. So the $(i,j)^{\text{th}}$ element in $\mathbf{A}_{m \times n}$ becomes the $(j,i)^{\text{th}}$ in the transpose $\mathbf{A}_{n \times m}^T$.

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}_{2 \times 3} \quad \mathbf{A}^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}_{3 \times 2}$$

- $(\mathbf{A}^T)^T = \mathbf{A}$
- $(\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$
- $(\mathbf{A} \mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T$
- $(c \cdot \mathbf{A})^T = c \cdot \mathbf{A}^T$

4. We can define matrix multiplication $\mathbf{A} \mathbf{B}$ if the number of elements in a row of \mathbf{A} is the same as the number of elements in the columns of \mathbf{B} . E.g. when \mathbf{A} is $(p \times k)$ and \mathbf{B} is $(k \times n)$. An element of the new matrix \mathbf{AB} is formed by taking the inner product of each row of \mathbf{A} with each column of \mathbf{B} . The matrix product \mathbf{AB} is

$$\mathbf{A}_{m \times n} \times \mathbf{B}_{n \times m} = \mathbf{C}_{m \times m} \text{ with } c_{ij} = \sum_{k=1}^n a_{ik} + b_{kj}$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \cdot \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11} \cdot b_{11} + a_{12} \cdot b_{21} & a_{11} \cdot b_{12} + a_{12} \cdot b_{22} \\ a_{21} \cdot b_{11} + a_{22} \cdot b_{21} & a_{21} \cdot b_{12} + a_{22} \cdot b_{22} \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}_{2 \times 3} \cdot \mathbf{A}^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}_{3 \times 2}$$

$$\mathbf{A} \mathbf{A}^T = \begin{bmatrix} 1(1) + 2(2) + 3(3) & 1(4) + 2(5) + 3(6) \\ 4(1) + 5(2) + 6(3) & 4(4) + 5(5) + 6(6) \end{bmatrix}_{2 \times 2}$$

- $(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$
- $\mathbf{A}(\mathbf{B}+\mathbf{C}) = \mathbf{AB}+\mathbf{AC}$
- $(\mathbf{A}+\mathbf{B})\mathbf{C} = \mathbf{AC}+\mathbf{BC}$
- \mathbf{AB} does not generally equal to \mathbf{BA} !

Special Square Matrix

1. A square matrix \mathbf{A} is said to be **symmetric** if $\mathbf{A} = \mathbf{A}^T$ or $a_{ij} = a_{ji}$ for all i and j .

$$\mathbf{A} = \begin{bmatrix} 3 & 5 \\ 5 & -2 \end{bmatrix}_{2 \times 2} \text{ is symmetric; } \quad \mathbf{A} = \begin{bmatrix} 3 & 5 \\ 6 & -2 \end{bmatrix}_{2 \times 2} \text{ is not symmetric}$$

$$2. \text{ Diagonal Matrix: } \mathbf{A}_{n \times n} = \text{diag}(a_1, \dots, a_n) = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & a_n \end{pmatrix}$$

$$3. \text{ Identity Matrix: } \mathbf{I}_{n \times n} = \text{diag}(\mathbf{1}_n) = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}$$

The identity matrix is a square matrix with ones on the diagonal and zeros elsewhere. It follows from the definition of matrix multiplication that the (i, j) entry of \mathbf{AI} is $a_{i1} \times 0 + \dots + a_{i,j-1} \times 0 + a_{ij} \times 1 + a_{i,j+1} \times 0 + \dots + a_{ik} \times 0 = a_{ij}$. So $\mathbf{AI} = \mathbf{A}$. Similarly, $\mathbf{IA} = \mathbf{A}$. Therefore matrix \mathbf{I} acts like 1 in ordinary multiplication.

The fundamental scalar relation about the existence of an inverse number a^{-1} such that $a^{-1} \cdot a = a \cdot a^{-1} = 1$, if $a \neq 0$, has the following matrix algebra extension.

$$\mathbf{B}_{k \times k} \mathbf{A}_{k \times k} = \mathbf{A}_{k \times k} \mathbf{B}_{k \times k} = \mathbf{I}_{k \times k}$$

then \mathbf{B} is called the inverse of \mathbf{A} and is denoted by \mathbf{A}^{-1} .

Other Matrix Properties

1. **Trace:** The sum of the diagonal elements, $\text{tr}(\mathbf{A}_{n \times n}) = \sum_{i=1}^n a_{ii}$.
2. A square matrix that does not have a matrix inverse is called a **singular** matrix. The inverse of a 2×2 matrix is given by

$$\mathbf{A}_{2 \times 2} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \quad \mathbf{A}_{2 \times 2}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

3. A matrix is singular if and only if its determinant is 0. The determinant of a matrix \mathbf{A} is denoted as $|\mathbf{A}|$. The determinant of a 2×2 matrix is given by

$$\mathbf{A}_{2 \times 2} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \det(\mathbf{A}) = ad - bc$$

Examples 1: Simultaneous equations

$$\begin{aligned} 5x + 3y + z &= 1 \\ 2x + 3y + 5z &= 2 \\ x + 9y + 6z &= 3 \end{aligned}$$

We can rewrite the above three equations as a single matrix equation:

$$\begin{bmatrix} 5 & 3 & 1 \\ 2 & 3 & 5 \\ 1 & 9 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Example 2: Variance/Covariance Matrix

For a vector of random variables, (Y_1, Y_2, \dots, Y_n) , we can write a matrix containing their variances and their covariances. Let σ_i^2 be the variance of Y_i and let cov_{ij} be the covariance between Y_i and Y_j , $i < j$. Then the variance/covariance matrix for (Y_1, Y_2, \dots, Y_n) is

$$\begin{bmatrix} \sigma_1^2 & cov_{12} & \dots & cov_{1n} \\ cov_{12} & \sigma_2^2 & \dots & cov_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ cov_{1n} & cov_{2n} & \dots & \sigma_n^2 \end{bmatrix}$$

Also note that the above can be written as

$$\begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix} \begin{bmatrix} 1 & \rho_{12} & \dots & \rho_{1n} \\ \rho_{12} & 1 & \dots & \rho_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1n} & \rho_{2n} & \dots & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}$$

where ρ_{ij} is the correlation of Y_i and Y_j . Note that all of these matrices are symmetric. Furthermore, the terms on the diagonal of the variance/covariance matrix must be positive and terms off the diagonal of the correlation matrix are bounded by -1 and 1.

Example 3: Multiple Linear Regression

We have a response Y and a set of p independent variables X_1, X_2, \dots, X_p . Assume we have n observations and for each $i = 1, \dots, n$ observation, we assume

$$Y_i = \beta_0 + \beta_1 x_{i,1} + \dots + \beta_p x_{i,p} + \varepsilon_i$$

where $\varepsilon_i \sim \text{Normal}(0, \sigma^2)$.

We can represent n observations simultaneously in matrix form as

$$\mathbf{Y}_{n \times 1} = \mathbf{X}_{n \times p+1} \boldsymbol{\beta}_{p+1 \times 1} + \boldsymbol{\varepsilon}_{n \times 1}$$

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots & \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

The residual $Y_i - (\beta_0 + \beta_1 x_{i,1} + \dots + \beta_p x_{i,p})$ can be written as

$$(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) = \begin{bmatrix} y_1 - (\beta_0 + \beta_1 x_{1,1} + \beta_2 x_{1,2} + \dots + \beta_p x_{1,p}) \\ y_2 - (\beta_0 + \beta_1 x_{2,1} + \beta_2 x_{2,2} + \dots + \beta_p x_{2,p}) \\ \vdots \\ y_n - (\beta_0 + \beta_1 x_{n,1} + \beta_2 x_{n,2} + \dots + \beta_p x_{n,p}) \end{bmatrix}_{n \times 1}$$

The residual sum of squares (RSS) is

$$\begin{aligned} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) &= \begin{bmatrix} y_1 - \beta_0 - \beta_1 x_{1,1} - \beta_2 x_{1,2} - \dots - \beta_p x_{1,p} \\ y_2 - \beta_0 - \beta_1 x_{2,1} - \beta_2 x_{2,2} - \dots - \beta_p x_{2,p} \\ \vdots \\ y_n - \beta_0 - \beta_1 x_{n,1} - \beta_2 x_{n,2} - \dots - \beta_p x_{n,p} \end{bmatrix}_{n \times 1}^T \\ &\quad \times \begin{bmatrix} y_1 - \beta_0 - \beta_1 x_{1,1} - \beta_2 x_{1,2} - \dots - \beta_p x_{1,p} \\ y_2 - \beta_0 - \beta_1 x_{2,1} - \beta_2 x_{2,2} - \dots - \beta_p x_{2,p} \\ \vdots \\ y_n - \beta_0 - \beta_1 x_{n,1} - \beta_2 x_{n,2} - \dots - \beta_p x_{n,p} \end{bmatrix}_{n \times 1} \\ &= \sum_{i=1}^n (Y_i - \beta_0 - \beta_1 x_{i,1} - \dots - \beta_p x_{i,p})^2 \end{aligned}$$

Minimizing the above RSS gives the usual least-squared estimate for $\boldsymbol{\beta}$

$$\hat{\boldsymbol{\beta}}_{OLS} = \operatorname{argmin}_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$