Matrix Algebra Formulae

Unit matrices

The unit matrix I of order n is a square matrix with all diagonal elements equal to one and all off-diagonal elements zero, i.e., $(I)_{ij} = \delta_{ij}$. If A is a square matrix of order n, then $AI = IA = A$. Also $I = I^{-1}$.
I is sometimes written as I_n if the order needs to be stated explicitly.

Products

If A is a $(n \times l)$ matrix and B is a $(l \times m)$ then the product AB is defined by

$$(AB)_{ij} = \sum_{k=1}^{l} A_{ik} B_{kj}$$

In general $AB \neq BA$.

Transpose matrices

If A is a matrix, then transpose matrix A^T is such that $(A^T)_{ij} = (A)_{ji}$.

Inverse matrices

If A is a square matrix with non-zero determinant, then its inverse A^{-1} is such that $AA^{-1} = A^{-1}A = I$.

$$(A^{-1})_{ij} = \frac{\text{transpose of cofactor of } A_{ij}}{|A|}$$

where the cofactor of A_{ij} is $(-1)^{i+j}$ times the determinant of the matrix A with the j-th row and i-th column deleted.

Determinants

If A is a square matrix then the determinant of A, $|A|$ ($\equiv \det A$) is defined by

$$|A| = \sum_{i,j,k,\ldots} \epsilon_{ijk\ldots} A_{1i} A_{2j} A_{3k} \ldots$$

where the number of the suffixes is equal to the order of the matrix.

2×2 matrices

If $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ then,

$$|A| = ad - bc \qquad A^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \qquad A^{-1} = \frac{1}{|A|} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Product rules

$$(AB \ldots N)^T = N^T \ldots B^T A^T$$

$$(AB \ldots N)^{-1} = N^{-1} \ldots B^{-1} A^{-1} \qquad \text{(if individual inverses exist)}$$

$$|AB \ldots N| = |A|\,|B| \ldots |N| \qquad \text{(if individual matrices are square)}$$

Orthogonal matrices

An orthogonal matrix Q is a square matrix whose columns q_i form a set of orthonormal vectors. For any orthogonal matrix Q,

$Q^{-1} = Q^T$, $\quad |Q| = \pm 1$, $\quad Q^T$ is also orthogonal.

Solving sets of linear simultaneous equations

If A is square then $A\boldsymbol{x} = \boldsymbol{b}$ has a unique solution $\boldsymbol{x} = A^{-1}\boldsymbol{b}$ if A^{-1} exists, i.e., if $|A| \neq 0$.

If A is square then $A\boldsymbol{x} = 0$ has a non-trivial solution if and only if $|A| = 0$.

An over-constrained set of equations $A\boldsymbol{x} = \boldsymbol{b}$ is one in which A has m rows and n columns, where m (the number of equations) is greater than n (the number of variables). The best solution x (in the sense that it minimizes the error $|A\boldsymbol{x} - \boldsymbol{b}|$) is the solution of the n equations $A^T A\boldsymbol{x} = A^T\boldsymbol{b}$. If the columns of A are orthonormal vectors then $\boldsymbol{x} = A^T\boldsymbol{b}$.

Hermitian matrices

The Hermitian conjugate of A is $A^\dagger = (A^*)^T$, where A^* is a matrix each of whose components is the complex conjugate of the corresponding components of A. If $A = A^\dagger$ then A is called a Hermitian matrix.

Eigenvalues and eigenvectors

The n eigenvalues λ_i and eigenvectors $\boldsymbol{u}_i$ of an $n \times n$ matrix A are the solutions of the equation $A\boldsymbol{u} = \lambda\boldsymbol{u}$. The eigenvalues are the zeros of the polynomial of degree n, $P_n(\lambda) = |A - \lambda I|$. If A is Hermitian then the eigenvalues λ_i are real and the eigenvectors u_i are mutually orthogonal. $|A - \lambda I| = 0$ is called the characteristic equation of the matrix A.

$$\mathrm{Tr}\, A = \sum_i \lambda_i, \quad \text{also } |A| = \prod_i \lambda_i.$$

If S is a symmetric matrix, Λ is the diagonal matrix whose diagonal elements are the eigenvalues of S, and U is the matrix whose columns are the normalized eigenvectors of A, then

$$U^T S U = \Lambda \qquad \text{and} \qquad S = U \Lambda U^T.$$

If x is an approximation to an eigenvector of A then $\boldsymbol{x}^T A\boldsymbol{x}/(\boldsymbol{x}^T\boldsymbol{x})$ (Rayleigh's quotient) is an approximation to the corresponding eigenvalue.

Commutators

$$[A, B] \equiv AB - BA$$
$$[A, B] = -[B, A]$$
$$[A, B]^\dagger = [B^\dagger, A^\dagger]$$
$$[A + B, C] = [A, C] + [B, C]$$
$$[AB, C] = A[B, C] + [A, C]B$$
$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

Hermitian algebra

$$\boldsymbol{b}^\dagger = (b_1^*, b_2^*, \ldots)$$

	Matrix form	Operator form	Bra-ket form
Hermiticity	$\boldsymbol{b}^* \cdot A \cdot \boldsymbol{c} = (A \cdot \boldsymbol{b})^* \cdot \boldsymbol{c}$	$\int \psi^* O \phi = \int (O\psi)^* \phi$	$\langle \psi \vert O \vert \phi \rangle$
Eigenvalues, λ real	$A\boldsymbol{u}_i = \lambda_{(i)} \boldsymbol{u}_i$	$O\psi_i = \lambda_{(i)} \psi_i$	$O \vert i \rangle = \lambda_i \vert i \rangle$
Orthogonality	$\boldsymbol{u}_i \cdot \boldsymbol{u}_j = 0$	$\int \psi_i^* \psi_j = 0$	$\langle i \vert j \rangle = 0 \quad (i \neq j)$

Completeness	$\boldsymbol{b} = \sum_i \boldsymbol{u}_i(\boldsymbol{u}_i \cdot \boldsymbol{b})$	$\phi = \sum_i \psi_i \left(\int \psi_i^* \phi \right)$	$\phi = \sum_i \|i\rangle \langle i\|\phi\rangle$
Rayleigh–Ritz			
Lowest eigenvalue	$\lambda_0 \leq \dfrac{\boldsymbol{b}^* \cdot A \cdot \boldsymbol{b}}{\boldsymbol{b}^* \cdot \boldsymbol{b}}$	$\lambda_0 \leq \dfrac{\int \psi^* O \psi}{\int \psi^* \psi}$	$\dfrac{\langle \psi\|O\|\psi\rangle}{\langle \psi\|\psi\rangle}$

Pauli spin matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\sigma_x \sigma_y = \mathrm{i}\sigma_z, \quad \sigma_y \sigma_z = \mathrm{i}\sigma_x, \quad \sigma_z \sigma_x = \mathrm{i}\sigma_y, \qquad \sigma_x \sigma_x = \sigma_y \sigma_y = \sigma_z \sigma_z = I$$