1. Operators and Matrices

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Operators

An operator is a symbol that stands for carrying out one or more mathematical operations on some function.

An operator is usually expressed by a letter with a hat (^) on top.

An operator always acts on a function from the left.
ex)

$$\hat{A} = x + \frac{d}{dx}, \; f(x) = a \sin bx \quad \rightarrow \quad \hat{A} f(x) = ax \sin bx + ab \cos bx.$$

On the other hand, the expression $f(x)\hat{A}$ is an operator multiplied by a function, which is still an operator.

Eigenfunctions and Eigenvalues

If a function f and an operator $\hat{A}$ satisfy the relation

$$\hat{A}f = af$$

where a is a constant, f and a are called an eigenfunction and an eigenvalue of the operator $\hat{A}$.

For an operator, there can be multiple (sometimes infinitely many) sets of eigenfunctions and eigenvalues.

The eigenvalues and eigenfunctions are the most important concepts for understanding the calculations regarding the quantum mechanics.

Operator Algebra

The addition and subtraction of an operator is defined as

$$\hat{C} = \hat{A} + \hat{B} \quad \rightarrow \quad \hat{C}f = \hat{A}f + \hat{B}f,$$
$$\hat{D} = \hat{A} - \hat{B} \quad \rightarrow \quad \hat{D}f = \hat{A}f - \hat{B}f.$$

When more than two operators are multiplied, the rightmost operator first acts to the function.

$$\hat{A}\hat{B}\hat{C}f = \hat{A}[\hat{B}(\hat{C}f)].$$

The commutator of two operators are defined as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A},$$

which is not necessarily zero – two operators are generally not commutative.

Operator Algebra

ex) Find the eigenfunctions of the operator $\dfrac{d}{dx}$.

ex) Evaluate the commutator $\left[x, \dfrac{d}{dx}\right]$.

Operator Algebra

An operator raised to a power is defined as successive multiplication of a same operator:

$$\hat{A}^2 = \hat{A}\hat{A}, \quad \hat{A}^3 = \hat{A}\hat{A}\hat{A}, \cdots$$

An inverse of an operator $\hat{A}^{-1}$ is defined as the operator that satisfies

$$\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I},$$

where $\hat{I}$ is an identity or unity operator that does nothing on a function (same as multiplication by 1).

Not all operators possess inverse.

Hermitian Operator

If an operator $\hat{A}$ satisfies

$$\int f^* \hat{A} g \, d\tau = \left(\int g^* \hat{A} f \, d\tau \right)^*$$

for arbitrary functions f and g, such operator is called Hermitian.

The notation

$$\int \langle \cdots \rangle \, d\tau$$

indicates integrating the function in $\langle \cdots \rangle$ over all space that it is defined. This allows us to use the same expressions in different dimensionalities.

Hermitian operators are important in quantum mechanics, as they are related to physical observables.

Matrix

A matrix is a list of quantities arranged in rows and columns.

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1n} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & A_{m3} & \cdots & A_{mn} \end{pmatrix}$$

The numbers $\{A_{mn}\}$are called matrix elements.

A matrix with m rows and n columns is called m-by-n matrix.

If $m = n$, the matrix is called a square matrix.

A single row and column are often called row vector and column vector, respectively, as they can be thought as one-dimensional arrays.

Matrix Algebra

A matrix is equal to another matrix if

- the number of rows and columns for the two matrices are identical,
- and all corresponding elements of the two matrices are also equal.

For two matrices

$$\mathbf{A} = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{pmatrix},$$

the addition and scalar multiplication is defined as

$$\mathbf{A} + \mathbf{B} = \begin{pmatrix} A_{11} + B_{11} & \cdots & A_{1n} + B_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} + B_{m1} & \cdots & A_{mn} + B_{mn} \end{pmatrix} \quad \text{and} \quad c\mathbf{A} = \begin{pmatrix} cA_{11} & \cdots & cA_{1n} \\ \vdots & \ddots & \vdots \\ cA_{m1} & \cdots & cA_{mn} \end{pmatrix}.$$

Matrix Algebra

The elements of the product matrix $\mathbf{C} = \mathbf{AB}$ is defined as

$$C_{mn} = \sum_k A_{mk} B_{kn}.$$

ex)

$$\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 2 & 1 \end{pmatrix} = ?$$

answer: $$\begin{pmatrix} 1\times 0 + 2\times 2 & 1\times 1 + 2\times 1 \\ 0\times 0 + 1\times 2 & 0\times 1 + 1\times 1 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 2 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 3 \\ 1 \end{pmatrix} = ?$$

answer: $$\begin{pmatrix} 1\times 0 + 0\times 3 + 2\times 1 \\ 0\times 0 + (-1)\times 3 + 1\times 1 \\ 0\times 0 + 0\times 3 + 1\times 1 \end{pmatrix} = \begin{pmatrix} 2 \\ -2 \\ 1 \end{pmatrix}$$

By definition, the multiplication can be only defined if the number of columns of $\mathbf{A}$ is equal to the number of rows of $\mathbf{B}$.

Matrix Algebra

Square matrices can be multiplied in any order, but they do not necessarily commute:

$$\mathbf{AB} \neq \mathbf{BA}.$$

Other than that, the matrix multiplication satisfies associativity and distributivity like scalars.

$$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC}),$$

$$\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}.$$

Example:

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Identity Matrix

An identity matrix $\mathbf{I}$ is a square matrix which satisfies

$$\mathbf{IA} = \mathbf{AI} = \mathbf{A},$$

and takes the form of

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}.$$

The elements can be summarized by using Kronecker delta δ_{ij},

$$I_{ij} = \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

Determinant

A square matrix $\mathbf{A}$ has a determinant $\det(\mathbf{A})$ which is a scalar.

For a 2-by-2 matrix, the determinant is

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \rightarrow \quad \det(\mathbf{A}) = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = A_{11}A_{22} - A_{12}A_{21}.$$

For higher-dimensional matrices, the determinants can be calculated by expansion by minors:

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = A_{11} \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} - A_{12} \begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} + A_{13} \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix}$$

$$= A_{11}A_{22}A_{33} - A_{11}A_{32}A_{23} - A_{12}A_{21}A_{33} + A_{12}A_{31}A_{23} + A_{13}A_{21}A_{32} - A_{13}A_{31}A_{22}.$$

Determinant

ex) Calculate the determinant

$$\begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix}.$$

Properties of Determinants

1.

$$\begin{vmatrix} 0 & 0 & 0 \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = 0, \quad \begin{vmatrix} 0 & A_{12} & A_{13} \\ 0 & A_{22} & A_{23} \\ 0 & A_{32} & A_{33} \end{vmatrix} = 0.$$

2.

$$\begin{vmatrix} A_{11} & A_{11} & A_{13} \\ A_{21} & A_{21} & A_{23} \\ A_{31} & A_{31} & A_{33} \end{vmatrix} = 0, \quad \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{11} & A_{12} & A_{13} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = 0.$$

3.

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = - \begin{vmatrix} A_{12} & A_{11} & A_{13} \\ A_{22} & A_{21} & A_{23} \\ A_{32} & A_{31} & A_{33} \end{vmatrix}, \quad \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = - \begin{vmatrix} A_{21} & A_{22} & A_{23} \\ A_{11} & A_{12} & A_{13} \\ A_{31} & A_{32} & A_{33} \end{vmatrix}.$$

Properties of Determinants

4.

$$\begin{vmatrix} cA_{11} & A_{12} & A_{13} \\ cA_{21} & A_{22} & A_{23} \\ cA_{31} & A_{32} & A_{33} \end{vmatrix} = c \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33}, \end{vmatrix},$$

$$\begin{vmatrix} cA_{11} & cA_{12} & cA_{13} \\ cA_{21} & cA_{22} & cA_{23} \\ cA_{31} & cA_{32} & cA_{33} \end{vmatrix} = c^3 \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33}, \end{vmatrix}.$$

5.

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = \begin{vmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{vmatrix}.$$

Linear Homogeneous Equations

Consider a set of linear simultaneous equation,

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= 0, \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= 0, \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= 0. \end{aligned}$$

$$\underbrace{\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_{\mathbf{x}} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

It is apparent that we have

$$x_1 = x_2 = x_3 = 0$$

as a solution of the problem, which is called the trivial solution. However, such a simple solution is usually not very interesting.

The condition for solutions other than trivial solution (nontrivial solution) is $\det(\mathbf{A}) = 0$.

Linear Homogeneous Equations

ex)

a.

$$4x + 5y = 0,$$
$$6x + 8y = 0.$$

$$\underbrace{\begin{pmatrix} 4 & 5 \\ 6 & 8 \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} x \\ y \end{pmatrix}}_{\mathbf{x}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\det(\mathbf{A}) = 4 \times 8 - 5 \times 6 = 2$$

b.

$$3x + 4y = 0,$$
$$6x + 8y = 0.$$

$$\underbrace{\begin{pmatrix} 3 & 4 \\ 6 & 8 \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} x \\ y \end{pmatrix}}_{\mathbf{x}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\det(\mathbf{A}) = 3 \times 8 - 4 \times 6 = 0$$