Eigenvalues and EigenVectors and Application of Linear Algebra in Quantum Mechanics

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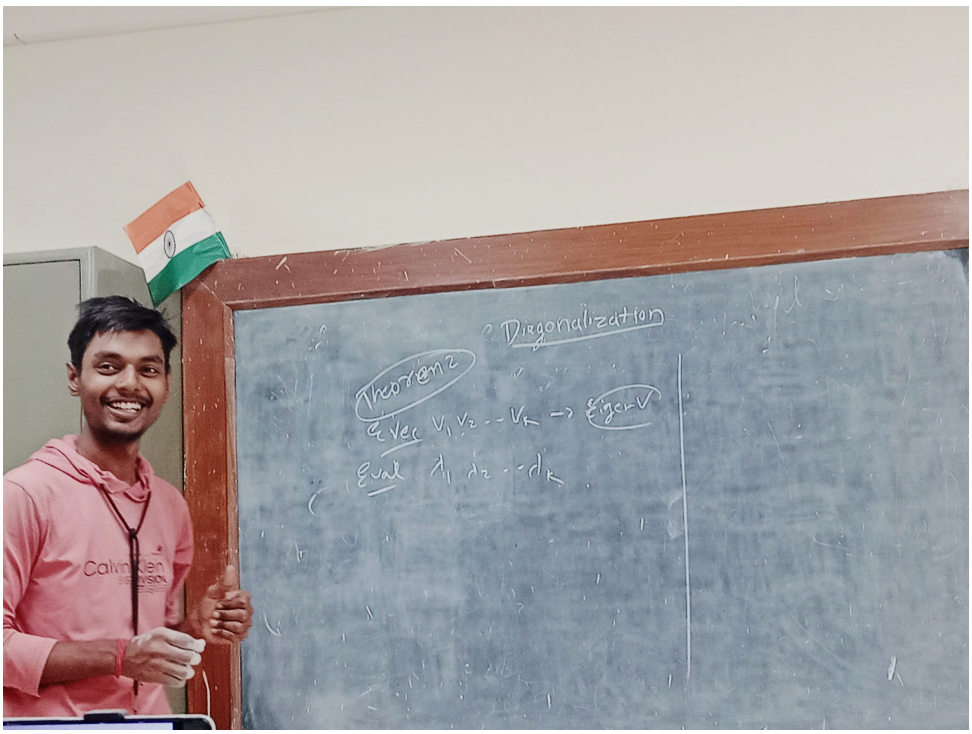
MLS01

Madhava Lecture Series, Theoretical Nexus



Krishnakant while Lecture

EigenValue Problem

In this section, we will look at a special situation where a given square matrix A and a vector x, the product Ax will be the same as the scalar multiplication λx for some scalar λ.

Review of Determinants

$$\det(A) = |A|$$

Solving 2×2 and 3×3 Determinants.

Some Situations

(i) If $\det(A) = 0$, **Singular Matrix**.

(ii) If $\det(A) \neq 0$, **Non-Singular Matrix**.

Cofactor, Minor, Inverse, Adjoint, Inverse.

If $n \times n$ Matrix, then:

(a) The only solution $Ax = 0$ is the **trivial solution** $(x = 0)$, if and only if $\det(A) \neq 0$.

(b) $Ax = 0$ will have **non-trivial solution**, if $\det(A) = 0$.

Eigenvalues & Vectors

$$\boxed{Ax = \lambda x}$$

This will not be possible for all vectors x, nor will it be possible for all scalars λ.

The goal of this section is to determine the vectors and scalars for which this will happen.

We will start with this definition:

Suppose $A \to n \times n$ matrix, x is a non-zero vector,

$$Ax = \lambda x$$

Then we will often call x the **Eigenvector** associated with λ (or we will call λ the **eigenvalue** corresponding to x associated with A).

$*$ They will occur in pairs.

What we need to figure out is just how can we determine eigenvectors and eigenvalues.

Start

1 Definition (1).

Given the equation:

$$A\mathbf{x} = \lambda\mathbf{x}$$

Rewriting it as:

$$A\mathbf{x} = \lambda I\mathbf{x}$$

we can write:

$$(\lambda I - A)\mathbf{x} = 0$$

If λ is an eigenvalue of A, this system must have a non-zero solution $\mathbf{x}$, and we know that $\mathbf{x}$ associated with λ cannot be the zero vector.

From the fundamental subspace section, we say that this system will have a non-zero solution if and only if:

$$\boxed{\det(\lambda I - A) = 0}$$

Thus, the eigenvalue will be the scalar for which the matrix $(\lambda I - A)$ is singular.

2 Defintion 2.

$$\det(\lambda I - A) = 0$$

This is called the characteristic equation of A.

When computed, it will be an n-th degree polynomial in λ of the form:

$$p(\lambda) = \lambda^n + C_{n-1}\lambda^{n-1} + \cdots + C_1\lambda + C_0$$

> Note that λ^n is the highest power, and the coefficient of λ^n is 1. Thus, this polynomial will have a degree of n.

Therefore, there will be n eigenvalues (possibly including repeats) because of the Fundamental Theorem of Algebra. An eigenvalue can repeat itself in the eigenvalue list.

To distinguish between eigenvalues (those that repeat and those that do not repeat), we will introduce ways of differentiation.

This will be discussed in the next section.

3 Definition 3.

Now Suppose:

Let A be an $m \times n$ matrix, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the list of eigenvalues, including repeats.

- If λ occurs once,
  $\lambda \rightarrow$ Simple Eigenvalue
- If λ occurs k times, $k \geq 2$,
  $\lambda \rightarrow$ It will have multiplicity of k.

Simple Method:

- Find $\lambda I - A$.
- $\det(\lambda I - A) = 0$
  You will get the characteristic polynomial.
- Find eigenvalues:
  - $\rightarrow$ Simple Eigenvalue
  - $\rightarrow$ Double Eigenvalue
  - $\rightarrow$ Triple Eigenvalue

Theorem 1:
Now we will calculate for Upper Triangular Matrix and Lower Triangular Matrix.

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}$$

- We will calculate $\det(\lambda I - A) = 0$.
- Solving that, we get the characteristic polynomial.

So we will get:

$$\boxed{\lambda_1 = a_1, \lambda_2 = a_2, \ldots, \lambda_n = a_n}$$

4 Definition 3.

The set of all solutions to $(A - \lambda I)X = 0$ is the **eigenspace** of A corresponding to λ.

There will be one eigenspace of A for each distinct value of λ, and so there will be from 1 to n eigenspaces.

Let us see with an example:
Matrix $A = \begin{bmatrix} 6 & 16 \\ -1 & -4 \end{bmatrix}$

$$(\lambda I - A)x = 0$$

Eigenvalues for this will be : $\lambda_1 = -2$ **&** $\lambda_2 = 4$
Now , finding EigenVectors :

$$\begin{bmatrix} -8 & -16 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

On solving this, the general solution for this:

$x_1 = -2t, \quad x_2 = t$

EigenVectors corresponding to $\lambda_1 = -2$

$$x = \begin{bmatrix} -2t \\ t \end{bmatrix} = t \begin{bmatrix} -2 \\ 1 \end{bmatrix}$$

We can see the basis here corresponding to $\lambda = -2$:

$$v_1 = \begin{bmatrix} -2 \\ 1 \end{bmatrix}$$

Same we will be doing with $\lambda_2 = 4$

$$v_2 = \begin{bmatrix} -8 \\ 1 \end{bmatrix}$$

$$\boxed{\lambda_1 = -2,\ v_1 = \begin{bmatrix} -2 \\ 1 \end{bmatrix},\ \lambda_2 = 4,\ v_2 = \begin{bmatrix} -8 \\ 1 \end{bmatrix}\ v_2 = \begin{bmatrix} -8 \\ 1 \end{bmatrix}}$$

if $\lambda$are same ,then only one Eigen Basis

5 Theorem

$\lambda$is a eigenvalue of the matrix A with corresponding eigenvectors x .
, then ,$\lambda^k$is an eigenvalue of the matrix A^k

$=\lambda^{k-1}(Ax)$
$= \lambda^{k-1}(\lambda x)$
$= \lambda^k x$

Theorem 3:

$A \to n \times n$ matrix
$\lambda_1, \lambda_2, \ldots, \lambda_n$ (including repetitions)

$$\det(A) = \lambda_1 \lambda_2 \ldots \lambda_n$$

$$\text{trace}(A)\,(\text{tr}(A)) = \lambda_1 + \lambda_2 + \ldots + \lambda_n$$

trace(A) is denoted by tr(A) is the sum of the entries on the main diagonal.

$$t(r)(A) = a_{11} + a_{22} + \ldots + a_{nn}$$

Proof: Rewriting characteristic polynomial,

$$\det(A - \lambda I) = (\lambda - \lambda_1)(\lambda - \lambda_2) \ldots (\lambda - \lambda_n)$$

For $\lambda \geq 0$, we get:

$$\det(-A) = (-\lambda_1)(-\lambda_2) \ldots (-\lambda_n)$$
$$\det(-A) = (-1)^n(\lambda_1 \lambda_2 \ldots \lambda_n)$$

From the properties of determinant:

$$\det(-A) = (-1)^n \det(A)$$

$$\det(A) = \lambda_1 \lambda_2 \lambda_3 \ldots \lambda_n$$

Diagonalization:

Square Matrix $\rightarrow$ diagonal matrix
Especially for tasks like:

- Calculating powers of matrices.
- Solving linear differential equations.

Def 1:
$A \rightarrow$ Square Matrix. $\exists$ invertible matrix P
such that $P^{-1}AP$ is a diagonal matrix.

We say that A is diagonalizable and P diagonalizes A.

Theorem 1:
$A \rightarrow n \times n$ matrix

(a) A is diagonalizable.

(b) A has n linearly independent eigenvectors.

a $\implies$ (b):
Proof: $A \rightarrow$ diagonalizable matrix
$P \rightarrow$ invertible matrix such that $P^{-1}AP$ is diagonal.

Let $P = [p_1, p_2, \ldots, p_n]$ be the columns, and
$D \rightarrow$ diagonal matrix.

$$\text{from } PDP^{-1} \implies D = P^{-1}AP$$

$$P = [p_1, p_2, \ldots, p_n],$$

$$D = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

(Pre-multiplication by P)

$$D = P^{-1}AP \implies AP = PD$$

$$A[p_1, p_2, \ldots, p_n] = [p_1, p_2, \ldots, p_n] \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

$$Ap_1 = \lambda_1 p_1, \quad Ap_2 = \lambda_2 p_2, \quad Ap_n = \lambda_n p_n$$

The diagonal entries $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues.

We note that:

- These are the set of linearly independent eigenvectors.
- We can go vice versa also (from (b) $\rightarrow$ (a)).

6 Theorem 2:

$v_1, v_2, \ldots, v_k$ are Eigen Vectors of A corresponding to k distinct Eigen values, i.e., $\lambda_1, \lambda_2, \ldots, \lambda_k$. Then the form is linearly independent set of vectors.

Proof:

Assume: $v_1, v_2, \ldots, v_k \rightarrow$ is a linearly dependent set.

So there will be $(v_1, v_2, \ldots, v_{p-1})$ as linearly independent set.

So if we go on to next vector $v_p + 1$, so will be linearly dependent set.

All scalars c_i will not be zero. So,

$$c_1 v_1 + c_2 v_2 + \cdots + c_p v_p + c_{p+1} v_{p+1} = 0 \tag{1}$$

Using their corresponding Eigen values:

$$c_1 \lambda_1 v_1 + c_2 \lambda_2 v_2 + c_3 \lambda_3 v_3 + \ldots \tag{2}$$

Multiplying λ_{p+1} both sides:

$$c_1 \lambda_{p+1} v_1 + c_2 \lambda_{p+1} v_2 + c_3 \lambda_{p+1} v_3 + \cdots = 0 \tag{3}$$

Subtracting (3) from (2):

We had assumed $\{v_1, v_2, \ldots, v_p\}$ linearly dependent but all scalar coefficients must all zero.

$$\begin{aligned} c_1(\lambda_1 - \lambda_{p+1}) &= 0 \\ c_2(\lambda_2 - \lambda_{p+1}) &= 0 \\ &\vdots \\ c_p(\lambda_p - \lambda_{p+1}) &= 0 \end{aligned}$$

$$c_1 = 0,\ c_2 = 0,\ \ldots,\ c_p = 0$$

We will get:

$$c_{p+1} = 0$$

Hence, all the scalars are zero.

So this linearly dependent set must be **wrong**.

7 Theorem 3.

$A \rightarrow n \times n$ Matrix.

If A has distinct Eigen values, then A is diagonalizable.

8 Theorem 4.

Suppose that A is a diagonalizable matrix and that

$$P^{-1}AP = D,$$

then:

(a) If k is any positive integer, we have

$$A^k = PD^kP^{-1}.$$

(b) If all diagonal entries of D are non-zero, then A is invertible:

$$A^{-1} = PD^{-1}P^{-1}.$$

Proof:

We will go with $k = 2$:

$$D^2 = (P^{-1}AP)^2$$
$$D^2 = (P^{-1}A)(PP^{-1})(AP)$$
$$D^2 = (P^{-1}AIAP)$$
$$D^2 = P^{-1}A^2P$$

Pre-multiplying by P & post-multiplying by P^{-1}:

$$A^2 = PD^2P^{-1}.$$

(b)

Since diagonal entries are non-zero, the diagonal matrix is invertible. We need to show that:

$$AC(PD^{-1}P^{-1}) = I.$$

Let $k = -1$:

$$A^{-1} = PD^{-1}P^{-1}.$$

For $k = 1$, we have:

$$A^k = PD^kP^{-1}.$$

Hence:

$$A^{-1} = PD^{-1}P^{-1}.$$

$$A(PD^{-1}P^{-1}) = (PDP^{-1})(PD^{-1}P^{-1}).$$

$$A = P(DD^{-1})P^{-1}.$$

$$P(DD^{-1})P^{-1} = PIP^{-1}.$$

$$PP^{-1} = I.$$

Application of Qauntum Mechanics

1. State Vectors and Hilbert Space

Hilbert Space

A **Hilbert space** is a mathematical construct where quantum states reside. It is a complete, infinite-dimensional complex vector space equipped with an inner product.

For example, for a particle in 1D space, the Hilbert space consists of square-integrable functions $\psi(x)$.

Quantum States as Vectors

A quantum state $|\psi\rangle$ is represented as a vector in the Hilbert space. For instance, the state of an electron might be:

$$|\psi\rangle = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

where a, b, c are complex numbers.

Superposition Principle

Quantum states can exist as linear combinations (superpositions) of basis states. If $|u\rangle$ and $|v\rangle$ are basis vectors, then:

$$|\psi\rangle = c_1|u\rangle + c_2|v\rangle$$

where c_1 and c_2 are complex coefficients.

Importance in Quantum Mechanics

- **Physical Systems**: Any physical system, such as a particle or atom, can be described by a vector in a Hilbert space.
- **Normalization**: Quantum states are normalized:

  $$\langle\psi|\psi\rangle = 1$$

  This ensures that probabilities derived from the state are meaningful.

Example: Two-State System

Imagine a particle in a system with two possible states $|0\rangle$ and $|1\rangle$ (e.g., a qubit in quantum computing). Its general state is:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where α, β are complex numbers, and:

$$|\alpha|^2 + |\beta|^2 = 1$$

2. Eigenvalues and Eigenvectors in Quantum Mechanics

What are Eigenvalues and Eigenvectors?

In linear algebra, given a linear operator $\hat{A}$ (or a square matrix), an eigenvector $|\psi\rangle$ and its corresponding eigenvalue λ satisfy the equation:

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle$$

where:

- $|\psi\rangle$ is a non-zero vector (eigenvector),
- λ is a scalar (eigenvalue),
- $\hat{A}$ is the operator or matrix.

Role in Quantum Mechanics

Eigenvalues and eigenvectors are crucial in quantum mechanics because:

- Physical observables, such as energy, position, and momentum, are represented by Hermitian operators.
- The measurement of an observable corresponds to an eigenvalue of the associated operator.
- After a measurement, the quantum state collapses to the corresponding eigenvector.

Example: Schrödinger's Equation

The time-independent Schrödinger equation is an eigenvalue problem:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

where:

- $\hat{H}$ is the Hamiltonian operator (total energy operator),
- E is the eigenvalue representing the energy of the system,
- $|\psi\rangle$ is the eigenvector representing the quantum state.

Matrix Representation

If $\hat{A}$ is represented as a 3×3 matrix:

$$\hat{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix},$$

then the eigenvalue equation becomes:

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle,$$

where:

$$|\psi\rangle = \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

Finding Eigenvalues

The eigenvalues are found by solving the characteristic equation:

$$\det(\hat{A} - \lambda I) = 0,$$

where I is the identity matrix.

Significance in Measurements

When measuring an observable $\hat{A}$:

- The possible outcomes are the eigenvalues of $\hat{A}$.
- The system's state collapses into the corresponding eigenvector $|\psi\rangle$.

Example: Spin Measurement

Consider the spin operator $\hat{S}_z$ for a spin-$\frac{1}{2}$ particle:

$$\hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The eigenvalues are $\pm\frac{\hbar}{2}$, corresponding to spin-up and spin-down states:

$$|\text{Spin-Up}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\text{Spin-Down}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

3. Inner Product and Probabilities in Quantum Mechanics

Inner Product in Hilbert Space

In quantum mechanics, the **inner product** is a key operation in Hilbert space, defined between two quantum states $|\psi\rangle$ and $|\phi\rangle$ as:

$$\langle\phi|\psi\rangle = \sum_i \phi_i^* \psi_i,$$

where:

- ϕ_i^* is the complex conjugate of the ith component of $|\phi\rangle$,
- ψ_i is the ith component of $|\psi\rangle$.

The inner product is a complex number and satisfies the following properties:

- **Linearity**: $\langle\phi|(\alpha|\psi\rangle + \beta|\chi\rangle) = \alpha\langle\phi|\psi\rangle + \beta\langle\phi|\chi\rangle$,
- **Conjugate Symmetry**: $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$,
- **Positive-Definiteness**: $\langle\psi|\psi\rangle \geq 0$, and $\langle\psi|\psi\rangle = 0$ if and only if $|\psi\rangle = 0$.

Connection to Probabilities

The inner product plays a crucial role in calculating probabilities in quantum mechanics:

$$P(\phi \to \psi) = |\langle \phi | \psi \rangle|^2,$$

where $P(\phi \to \psi)$ is the probability of transitioning from the state $|\phi\rangle$ to the state $|\psi\rangle$. Here:

- $\langle \phi | \psi \rangle$ is the probability amplitude (a complex number),
- $|\langle \phi | \psi \rangle|^2$ is the modulus squared of the amplitude, which is a real number between 0 and 1.

Normalization Condition

Quantum states must be normalized to ensure meaningful probabilities:

$$\langle \psi | \psi \rangle = 1.$$

Example: Superposition State

Consider a quantum state in a two-level system:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle,$$

where $|0\rangle$ and $|1\rangle$ are basis states, and $\alpha, \beta \in \mathbb{C}$. The normalization condition requires:

$$|\alpha|^2 + |\beta|^2 = 1.$$

If a measurement is made to determine the system's state, the probabilities are:

- Probability of $|0\rangle$: $P(0) = |\langle 0 | \psi \rangle|^2 = |\alpha|^2$,
- Probability of $|1\rangle$: $P(1) = |\langle 1 | \psi \rangle|^2 = |\beta|^2$.

Orthogonality and Measurement

States $|u\rangle$ and $|v\rangle$ are **orthogonal** if:

$$\langle u | v \rangle = 0.$$

Orthogonal states represent mutually exclusive measurement outcomes.

Example: Spin-$\frac{1}{2}$ System

For a spin-$\frac{1}{2}$ particle, consider the spin states:

$$|\text{Up}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\text{Down}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The inner product between these states is:

$$\langle \text{Up} | \text{Down} \rangle = 0,$$

indicating orthogonality.

4. Expectation Value in Quantum Mechanics

Definition of Expectation Value

The **expectation value** of an observable $\hat{A}$ in a quantum state $|\psi\rangle$ is the average value of repeated measurements of $\hat{A}$ on a system in the state $|\psi\rangle$. It is given by:

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle,$$

where:

- $|\psi\rangle$ is the quantum state (a normalized vector in the Hilbert space),
- $\hat{A}$ is the Hermitian operator representing the observable,
- $\langle \psi | \hat{A} | \psi \rangle$ is a scalar value.

Properties of the Expectation Value

1. **Real Values**: Since $\hat{A}$ is a Hermitian operator, the expectation value $\langle \hat{A} \rangle$ is always real. 2. **Normalization Requirement**: The state $|\psi\rangle$ must be normalized:

$$\langle \psi | \psi \rangle = 1.$$

3. **Linearity**: If $|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$, then:

$$\langle \hat{A} \rangle = |c_1|^2 \langle \phi_1 | \hat{A} | \phi_1 \rangle + |c_2|^2 \langle \phi_2 | \hat{A} | \phi_2 \rangle.$$

Connection to Measurements

The expectation value does not predict individual measurement results but represents the statistical average of many measurements of $\hat{A}$ on identically prepared systems.

Example: Position Expectation Value

For a particle in a state $|\psi\rangle$, the position operator $\hat{x}$ has the expectation value:

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) \, dx,$$

where $\psi(x)$ is the wavefunction, and $\psi^*(x)$ is its complex conjugate.

Example: Energy Expectation Value

For the Hamiltonian operator $\hat{H}$, representing the total energy of a system, the expectation value is:

$$\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle.$$

This gives the average energy of the system in the state $|\psi\rangle$.

Matrix Representation

If $|\psi\rangle$ and $\hat{A}$ are represented in matrix form:

$$|\psi\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix},$$

then the expectation value is:

$$\langle \hat{A} \rangle = \begin{bmatrix} \psi_1^* & \psi_2^* & \psi_3^* \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix}.$$

Variance and Uncertainty

The variance of an observable $\hat{A}$ in the state $|\psi\rangle$ is given by:

$$\text{Var}(\hat{A}) = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2.$$

This quantifies the spread of measurement outcomes and is related to the Heisenberg uncertainty principle.

Other Uses of Linear Algebra in Quantum Mechanics

1. **Unitary Transformations**
2. **Tensor Product for Multi-Particle Systems**
3. **Quantum Computation**
4. **Diagonalization in Measurement Theory**
5. **Probability and Inner Product Spaces**

Conclusion

Linear algebra serves as the mathematical backbone of quantum mechanics, enabling a precise description of quantum states, observables, and their interactions. Concepts such as state vectors, eigenvalues, eigenvectors, inner products, and expectation values are integral to understanding quantum systems and predicting measurement outcomes. By leveraging these mathematical tools, physicists gain deep insights into the probabilistic nature of the quantum world, bridging the gap between abstract theory and experimental observations.