



## Spectral Decomposition I

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ABSTRACT: References are of course my favorite [1, 2] and additionally, [3–5]. I find [6] is very good. The goal is to understand the reason for finding eigenvalues and eigenvectors in physics.

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Last time, we learnt that the important thing is invariant under the basis. Then there is no reason to work in the complicated basis. We want the most simple matrix expression of linear map.

## 1 Invariant subspace

When we solve the problem, if it is possible, we divide it into the small independent parts and solve each part independently. For example, let us see the 3D projectile motion we learnt when we were freshman. We first find the plane of particle moving, and neglect the direction perpendicular to that plane. In remaining 2D motion, we again divide the motion into the two one-dimensional motion which are perpendicular and parallel to the acceleration. We solve each direction independently, and have said that projectile motion is a motion which has a uniform velocity in the direction perpendicular to the acceleration and uniform acceleration in the direction parallel to the acceleration. Therefore, we want to tell the process of dividing vector space into the subspaces and solving problem in that subspaces.

In other words, we want the operator which allow us to pick out the subspace part from the vector. If it is just picking out the subspace part, repeated application of it does not affect the result.

**Definition 1.1.** Idempotent An operator  $P \in \text{End}(V)$  is called *idempotent* if

$$P = PP := P \circ P. \quad (1.1)$$

Its matrix representation  $\mathbf{P} \in \text{Mat}_n(\mathbb{K})$  is called *idempotent matrix* and  $\mathbf{P}\mathbf{P} = \mathbf{P}$ .

### Box 1.1: Complete Orthonormal Set of Idempotents

Let the vector space  $V$  decomposed into  $r$  subspaces,

$$V = U_1 \oplus U_2 \oplus \dots \oplus U_r = \bigoplus_{i=1}^r U_i. \quad (1.2)$$

Let  $P_j \in \text{End}(V)$ ,  $j \in \{1, \dots, r\}$  be an idempotent operator such that

$$P_j : V \rightarrow V \quad \text{by } |v\rangle \mapsto |v_j\rangle \in U_j, \quad (1.3)$$

where  $|v\rangle = \sum_j |v_j\rangle$  and  $\forall j \in \{1, \dots, r\} : |v_j\rangle \in U_j$ . Then  $\{P_j\}_{i=1}^r$  is a *complete set of orthogonal idempotents*, that is

$$P_i P_j = \delta_{ij} P_j \quad (\text{no sum}), \quad \sum_{j=1}^r P_j = \mathbb{1}. \quad (1.4)$$

*Proof.* Let us first check the orthonormality: For  $i = j$ ,

$$|P_j P_j v\rangle = |P_j v_j\rangle = |v_j\rangle = |P_j v\rangle. \quad (1.5)$$

For  $i \neq j$ , since  $U_i \cap U_j = \emptyset$ ,

$$|P_i P_j v\rangle = |P_i v_j\rangle = 0. \quad (1.6)$$

For the completeness,

$$|v\rangle = \sum_j |v_j\rangle = \sum_j |P_j v\rangle = \left| \sum_j P_j v \right\rangle. \quad (1.7)$$

Therefore,  $\sum_j P_j = \mathbf{1}$ <sup>1</sup>. □

**Theorem 1.1.** The completeness implies

$$\forall T \in \text{End}(V) : T = \sum_j T_j \quad \text{where } T_j := P_j T \in \text{End}(U_j) \quad (1.8)$$

In the inner product space, we could define more concepts which are useful in physics.

**Box 1.2: Projection Operator**

Let  $V$  be an inner product space, then  $P \in \text{End}(V)$  is called a *projection* operator on  $V$  if it is *Hermitian idempotent*.

**Theorem 1.2.** Let  $P_1, P_2$  be a projection operators. Then  $P_1 + P_2$  is a projection operator iff  $P_1 \perp P_2$ .

*Proof.* It should be idempotents:

$$(P_1 + P_2)^2 = P_1^2 + P_1 P_2 + P_2 P_1 + P_2^2 = P_1 + P_1 P_2 + P_2 P_1 + P_2 = P_1 + P_2. \quad (1.9)$$

Therefore,

$$P_1 P_2 + P_2 P_1 = 0. \quad (1.10)$$

On the other hand, applying  $P_1$  on left/right yields

$$P_1 P_2 P_1 + P_1 P_2 = 0, \quad P_1 P_2 P_1 + P_2 P_1 = 0. \quad (1.11)$$

Subtracting those equations results

$$P_1 P_2 - P_2 P_1 = 0 \quad (1.12)$$

From Eq. (1.10) and Eq. (1.12), we obtain

$$P_1 P_2 = 0. \quad (1.13)$$

Using the inner product of endomorphisms  $g$ ,

$$g(P_1, P_2) = \text{tr}(P_1^\dagger P_2) = \text{tr}(P_1 P_2) = \text{tr} 0 = 0. \quad (1.14)$$

By definition, they are orthogonal. □

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<sup>1</sup>This is an extension of the concept of completeness of basis

Using projection operator, we can divide the space into the space we want to solve “now” and “later”.

**Definition 1.2** (Orthogonal Complement). Let  $V$  be an inner product space and  $U \subseteq V$  be a subspace of  $V$ . Then, the *orthogonal complement* of  $U$ , denoted  $U^\perp$  is

$$U^\perp = \{|v\rangle \in V \mid \forall |u\rangle \in U : \langle u|v\rangle = 0\}. \quad (1.15)$$

**Theorem 1.3.** Let  $U$  be the subspace of inner product space  $V$ . Then  $U^\perp$  is also a subspace of  $V$ .

*Proof.* We need to check

$$\forall a \in \mathbb{K} : \forall |v_1\rangle, |v_2\rangle \in U^\perp : a|v_1\rangle + |v_2\rangle \in U^\perp. \quad (1.16)$$

If  $|u\rangle \in U$ . Then,  $\forall |v_1\rangle, |v_2\rangle \in U^\perp :$

$$\langle u|av_1 + v_2\rangle = a\langle u|v_1\rangle + \langle u|v_2\rangle = 0. \quad (1.17)$$

Therefore,  $a|v_1\rangle + |v_2\rangle \in U^\perp$  □

**Lemma 1.4.** If  $U \subseteq V$  is a subspace of inner product space  $V$ ,

$$V = U \oplus U^\perp. \quad (1.18)$$

**Lemma 1.5.** Let  $U \subseteq V$  is a subspace of inner product space  $V$ . If  $P$  is a projection operator on  $V$  such that  $\forall |v\rangle \in V : |Pv\rangle \in U$ , the operator  $\mathbb{1} - P$  is a projection operator on  $V$  which maps to the vector into the orthogonal complement of  $U$ . That is,

$$|v\rangle = |(P + \mathbb{1} - P)v\rangle = |Pv\rangle + |(\mathbb{1} - P)v\rangle \quad (1.19)$$

where  $|Pv\rangle \in U$ ,  $|(\mathbb{1} - P)v\rangle \in U^\perp$ .

Now we know how to divide vector spaces. We just apply the projection operator to the vector space. The next question we can ask is then what subspace make the problem simple (or independent) to solve?

#### Box 1.3: Invariant Subspace

Let  $A \in \text{End}(V)$ . A subspace  $U \subseteq V$  is called an *invariant subspace* of  $A$  or *A-invariant* iff

$$\forall |u\rangle \in U : |Au\rangle \in U. \quad (1.20)$$

We write  $A(U) \subseteq U$ .

#### Box 1.4: Reduce

Let  $A \in \text{End}(V)$ . If  $U$  and  $U^\perp$  are both invariant subspace of  $A$ , we call  $U$  *reduces*  $A$ .

**Lemma 1.6.** If  $U$  is invariant under  $A$ , then  $U^\perp$  is invariant under  $A^\dagger$ .

*Proof.* Let  $|v\rangle \in U^\perp$ . Then, by definition,

$$\forall |u\rangle \in U : \quad \langle u|v\rangle = 0. \quad (1.21)$$

And because  $U$  is invariant under  $A$ ,  $|Au\rangle \in U$ . Therefore,

$$\langle u|A^\dagger v\rangle = \langle Au|v\rangle = 0. \quad (1.22)$$

Hence,  $|A^\dagger v\rangle \in U^\perp$ .  $\square$

**Lemma 1.7.** A subspace  $U \subseteq V$  reduces  $A$  iff it is invariant under  $A$  and  $A^\dagger$ .

**Theorem 1.8.** Let  $U \subseteq V$  be an invariant subspace of  $A$ . Let  $\{|e_i\rangle\}_{i=1}^{\dim U}$  be the basis of  $U$  and  $\{|e_i\rangle\}_{i=\dim U+1}^{\dim V}$  be the basis of  $U^\perp$ . Then, a matrix representation of  $A \in \text{End}(V)$ ,  $\mathbf{A}$  is the block matrix of the form

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{0} & \mathbf{A}_{22} \end{pmatrix}. \quad (1.23)$$

We say that  $\mathbf{A}_{11}$  represents  $\mathbf{A}$  in  $U$ .

*Proof.* In the given basis, the vector  $|u\rangle \in U$  can be represented in the column vector  $|u\rangle = (u^1, u^2, \dots, u^{\dim U}, 0, 0, \dots, 0)^\top = (\mathbf{u}^\top, \mathbf{0})^\top$ <sup>2</sup>. Therefore,

$$|Av\rangle = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{0} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11}\mathbf{u} \\ \mathbf{0} \end{pmatrix}. \quad (1.24)$$

$\square$

Moreover, if  $U$  reduces  $A$ , its matrix representation can be written in the *block-diagonal* form

**Theorem 1.9.** Let  $U \subseteq V$  be an invariant subspace of  $A$ . Let  $\{|e_i\rangle\}_{i=1}^{\dim U}$  be the basis of  $U$  and  $\{|e_i\rangle\}_{i=\dim U+1}^{\dim V}$  be the basis of  $U^\perp$ . Then, a matrix representation of  $A \in \text{End}(V)$ ,  $\mathbf{A}$  is the block matrix of the form

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 \end{pmatrix}. \quad (1.25)$$

This form is called *block-diagonal* form and we write  $\mathbf{A} = \mathbf{A}_1 \oplus \mathbf{A}_2$ .

**Definition 1.3.** If there is a suitable choice of basis which makes the matrix representation of  $A \in \text{End}(V)$ ,  $\mathbf{A}$ , we call  $\mathbf{A}$  is a *reducible representation*. Otherwise, it is called *irreducible representation*.

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<sup>2</sup>I believe that there is no confusion for using the same notation  $\mathbf{0}$  for zero matrix and vector. One can always check its dimension by checking the dimension of nonzero parts.

**Lemma 1.10.** Let  $U \subseteq V$  be a subspace of inner product space  $V$  and  $P$  be a projection operator on  $V$  onto  $U$ . Then,  $U$  is invariant under  $A$  iff  $AP = PAP$ .

*Proof.* ( $\Leftarrow$ )

Let  $|Pv\rangle = |u\rangle \in U$ .

$$|APv\rangle = |Au\rangle = \quad (1.26)$$

Since  $PAP = AP$ ,

$$|Au\rangle = |PAu\rangle. \quad (1.27)$$

In other words,  $|Au\rangle \in U$ . Therefore,  $U$  is invariant under  $A$ .

( $\Rightarrow$ ) Since  $U$  is invariant under  $A$ ,

$$\forall |u\rangle \in U : |Au\rangle \in U. \quad (1.28)$$

Since  $\forall v \in V : |Pv\rangle \in U$ ,

$$|APv\rangle \in U. \quad (1.29)$$

Since projection does not change the vector in  $U$ ,

$$\forall v \in V : |PAPv\rangle = |APv\rangle. \quad (1.30)$$

We conclude that  $PAP = AP$ .  $\square$

**Lemma 1.11.**  $U$  reduces  $A$  iff  $PA = AP$ .

*Proof.*

$$\begin{aligned} U \text{ reduces } A &\iff U \text{ is a subspace of both } A \text{ and } A^\dagger \\ &\iff ((AP = PAP) \wedge (A^\dagger P = PA^\dagger P)) \\ &\iff ((AP = PAP) \wedge (P^\dagger A = P^\dagger AP^\dagger)) \\ &\iff ((AP = PAP) \wedge (PA = PAP)) \\ &\iff (AP = PA) \end{aligned}$$

Note that  $AP = PA$  implies  $AP = PAP$ .  $\square$

## 2 Eigenvalues and Eigenvectors

The simplest invariant subspace is one-dimensional subspace. To find it, we define following.

### Box 2.1: Eigenvalues and Eigenvectors

Let  $V$  be a  $\mathbb{K}$ -vector space and  $A \in \text{End}(V)$ . Then a scalar  $a \in \mathbb{K}$  is called an *eigenvalue* if

$$\exists |v\rangle \in (V \setminus \{|v\rangle\}) : |Av\rangle = a|v\rangle. \quad (2.1)$$

The vector  $|v\rangle$  is called an *eigenvector* corresponding to eigenvalue  $a$ .

*Remark.* Note that the eigenvectors does not contain  $|0\rangle$ . We do not include it because it is trivial. But consequently, set of all eigenvectors corresponding to certain eigenvector is not a vector space.

**Definition 2.1** (Eigenspace). The set of zero vector and all eigenvectors corresponding to eigenvalue  $a$  is called an *eigenspace* of  $A$  corresponding to  $a$ . Let us write  $E_a$

$$E_a := \{|0\rangle\} \cup \{|v\rangle \in V \mid |Av\rangle = a|v\rangle\}. \quad (2.2)$$

**Theorem 2.1.** The eigenspace  $E_a \subseteq V$  of  $A$  is invariant subspace of  $A$ .

**Definition 2.2** (geometric multiplicity). Let  $E_a$  be a eigenspace of  $A$  corresponding to  $a$ .  $\dim E_a$  is called a *geometric multiplicity* of  $a$ . If  $\dim E_a = 1$ , we call  $a$  is simple.

#### Box 2.2: Spectrum

The set of eigenvalues of  $A \in \text{End}(V)$  is called a *spectrum* of  $A$ .

**Theorem 2.2** (orthogonality of eigenspace). If  $a \neq b$ ,  $E_a \cap E_b = \{|0\rangle\}$ .

*Proof.* If  $|v\rangle \in E_a \cap E_b$ , by definition,

$$a|v\rangle = |Av\rangle = b|v\rangle. \quad (2.3)$$

Therefore,

$$(b - a)|v\rangle = 0. \quad (2.4)$$

Since  $b \neq a$ ,

$$|v\rangle = 0 = |0\rangle. \quad (2.5)$$

□

**Lemma 2.3.** Let  $\{a_i\}_{i=1}^r$  be the set of distinct eigenvalues of  $A$  and  $E_{a_i}$  are the eigenspace for each eigenvalues. Then,

$$E_{a_1} + \dots + E_{a_r} = E_{a_1} \oplus \dots \oplus E_{a_r} = \bigoplus_{i=1}^r E_{a_i}. \quad (2.6)$$

**Lemma 2.4.** Let  $\{a_i\}_{i=1}^r$  be the set of all distinct eigenvalues of  $A$  and  $E_{a_i}$  are the eigenspace for each eigenvalues. Then,

$$\bigoplus_{i=1}^r E_{a_i} \subseteq V \quad (2.7)$$

is the invariant subspace of  $A$ .

**Lemma 2.5.** The number of eigenvalues  $\leq \dim V$ .

*Proof.* Because  $\dim E_{a_i} \geq 1$ ,

$$r \leq \sum_{i=1}^r \dim E_{a_i} = \dim \left( \bigoplus_{i=1}^r E_{a_i} \right) \leq \dim V. \quad (2.8)$$

□

Now we are happy that because we have invariant subspace when we find the eigenvalues and eigenspaces. On the other hand, how to find it? The answer goes back to the definition. We just transpose the r.h.s. to the l.h.s. of eigenvalue equation:

$$|(A - a\mathbb{1})v\rangle = 0. \quad (2.9)$$

Note that identity map  $\mathbb{1} \in \text{End}(V)$  is specified to show multiplying  $a$  is also endomorphism. Recall that we have nontrivial solution, that is nonzero  $|v\rangle$  satisfying above equation when there is no inverse of  $(A - a\mathbb{1})$ . Recall also that

$$\nexists (A - a\mathbb{1})^{-1} \iff \det(A - a\mathbb{1}) = 0. \quad (2.10)$$

Recall that the determinant of endomorphism is the determinant of a matrix representation of that endomorphism. Therefore, it is a polynomial of degree  $\dim V$ .

#### Box 2.3: Characteristic Polynomial and Characteristic Root

Let  $A \in \text{End}(V)$ . The polynomial  $\det(A - a\mathbb{1})$  is called a *characteristic polynomial*. And the root of the polynomial equation  $\det(A - a\mathbb{1}) = 0$  is called the *characteristic root*.

There is a famous theorem (we will not prove) that called fundamental theorem of algebra. It has many equivalent statements. For us, the following statement is the most suitable.

**Theorem 2.6** (Fundamental Theorem of Algebra). Every non-zero, single-variable, degree  $n$  polynomial with complex coefficients has, counted with algebraic multiplicity, exactly  $n$  complex roots. That is, polynomial of  $x$  with degree  $n$  can always be factorised in the form

$$c(x - a_1) \dots (x - a_n). \quad (2.11)$$

**Definition 2.3** (Algebraic multiplicity). If the same factor appears  $s$  times, we call its algebraic multiplicity is  $s$ . For example, in the above factorisation let us say  $a_1 = a_2 = \dots = a_s < a_{s+1} \leq a_{s+2} \dots \leq a_n$ . Then, we say the algebraic multiplicity of  $a_1$  is  $s$ .

Note that we have at least one root (with multiplicity  $n$ .) As a direct consequence, for the characteristic polynomial, we have the following theorem.

**Theorem 2.7.** Let  $A \in \text{End}(V)$ . It has at least one eigenvalue and therefore, at least one eigenvector.

**Theorem 2.8.** Let  $A \in \text{End}(V)$  and  $\{a_i\}_{i=1}^r$  be the set of eigenvalues of  $A$ . Let the algebraic multiplicity of  $a_i$  be  $m_i$ . Then,

$$\det A = \prod_{i=1}^r a_i^{m_i} \quad (2.12)$$

**Lemma 2.9.** Let  $A \in \text{End}(V)$  and  $\{a_i\}_{i=1}^r$  be the set of eigenvalues of  $A$ .

$$\exists A^{-1} \iff \forall i \in \{1, \dots, r\} : a_i \neq 0. \quad (2.13)$$

**Example 2.9.1** (Eigenvalue of Projection operator). Let  $P \in \text{End}(V)$  be a projection operator and  $|v\rangle$  be an eigenvector of  $P$  having eigenvalue  $p$ :

$$|Pv\rangle = p|v\rangle. \quad (2.14)$$

Then,

$$\begin{aligned} |P^2v\rangle &= p|Pv\rangle = p^2|v\rangle \\ &= |Pv\rangle = p|v\rangle. \end{aligned}$$

In the second line, we use the fact that  $P$  is idempotent. Therefore,

$$(p^2 - p)|v\rangle = 0. \quad (2.15)$$

By definition,  $|v\rangle \neq 0$ . Therefore  $p^2 - p = 0$ . Therefore, the projection operator can have eigenvalues 1 or 0. In general, if  $P \neq 1$ , it has eigenvalue 0 and it is not invertible.

Recall that the determinant is basis independent. The eigenvalue is also basis independent.

**Lemma 2.10.** If  $A, B \in \text{Mat}_n(\mathbb{K})$  are similar, they have the same eigenvalues.

*Proof.* The characteristic equation is

$$\begin{aligned} \det(\mathbf{B} - \lambda \mathbf{1}) &= \det(\mathbf{SAS}^{-1} - \lambda \mathbf{1}) \\ &= \det(\mathbf{SAS}^{-1} - \mathbf{S}\lambda \mathbf{1}\mathbf{S}^{-1}) \\ &= \det[\mathbf{S}(A - \lambda \mathbf{1})\mathbf{S}^{-1}] \\ &= \det(A - \lambda \mathbf{1}) \end{aligned}$$

Therefore,  $\mathbf{A}$  and  $\mathbf{B}$  has the same eigenvalue. □

Recall that the determinant of diagonal operator (more generally, upper triangular matrix) is just the multiplication of its diagonal elements. Therefore, if it is possible to work with the basis whose matrix representation of the endomorphism diagonal, it will be the best.

**Definition 2.4** (Diagonalisable). An operator  $A \in \text{End}(V)$  is called *diagonalisable* if the set of linearly independent eigenvectors form a basis set.

**Theorem 2.11.** If  $A \in \text{End}(V)$  is diagonalisable, there is a complete orthonormal set of projection operators  $\{P_j\}$  such that

$$A = \sum_j \lambda_j P_j. \quad (2.16)$$

*Proof.* We can construct such a projection operator directly. Let  $\{|e_i^{(j)}\rangle\}_{j=1}^{m_j}$  be the basis corresponding to the  $a_i$  with multiplicity  $m_j$ . Then,

$$P_i = \sum_{j=1}^{m_j} |e_i^{(j)}\rangle \langle e_i^{(j)}| \quad (2.17)$$

works. □

**Theorem 2.12.** Let  $A \in \text{End}(V)$  and  $\{a_i\}_{i=1}^r$  be the eigenvalue set of  $A$ . Let  $E_i$  be the eigenspace corresponding to the eigenvalue  $a_i$ . The following are equivalent:

- $A$  is diagonalisable.
- $V$  has a basis of eigenvectors for  $A$ .
- $V = \bigoplus_{i=1}^r E_i$
- $\dim V = \sum_{i=1}^r \dim E_i$

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