計算科学・量子計算における情報圧縮

Data Compression in Computational Science and Quantum Computing

2022.10.13

#2:線形代数の復習

Review of linear algebra

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Outline

- Review of linear algebra
  - Vector space- Abstract vectors-
    - General vector space (with inner product)
    - Basis and relation to coordinate vector space
    - Vector subspace and spanned vector subspace
  - Matrix and linear map
    - Relation between matrices and linear maps
  - Eigenvalue problem and diagonalization

Review of linear algebra

Vector space -Abstract vectors-

A quantum state is a **vector**

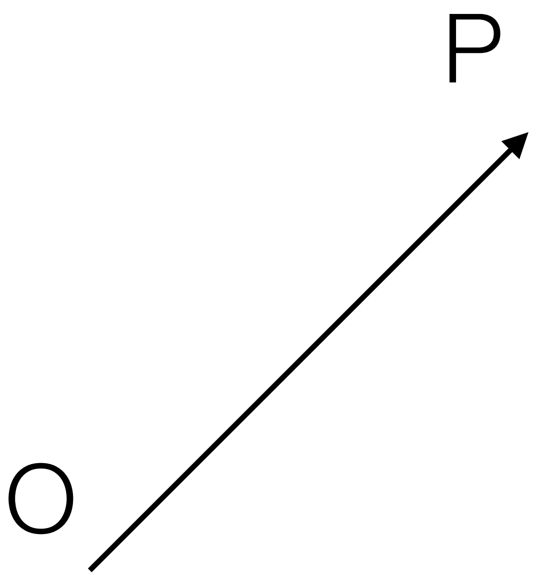
$$|\Psi\rangle$$

Geometric vector

Geometric vector: Arrow on the plane (or the space) ,

which has "Direction" and "Length"

$$\vec{v} \equiv \overrightarrow{OP}$$



We can express a vector by its component:

$$\vec{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} x_p - x_o \\ y_p - y_o \\ z_p - z_o \end{pmatrix}$$

Inner product of vector

Inner product:

$$(\vec{a},\vec{b}) \equiv \vec{a}\cdot\vec{b}$$

$$= a_x b_x + a_y b_y + a_z b_z$$

Example:

$$\vec{a} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}, \vec{b} = \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix}$$

Properties:

$$(\vec{a},\vec{a}) \geq 0$$

$$(\vec{a},\vec{b}) = (\vec{b},\vec{a})$$

$$(\vec{a}+\vec{b},\vec{c}) = (\vec{a},\vec{c}) + (\vec{b},\vec{c})$$

$$(c\vec{a},\vec{b}) = c(\vec{a},\vec{b}) \qquad c \in \mathbb{R}$$

Norm (length):

$$\|\vec{a}\| \equiv \sqrt{(\vec{a},\vec{a})}$$

Vector space (linear space)

Vector space $\mathbb{V}$: generalization of geometric vector

Set of elements (vectors) satisfying following **axioms**（公理）

Properties of addition:

$$\vec{a} + \vec{b} = \vec{b} + \vec{a}$$ Commutative property（交換法則）

$$\left(\vec{a} + \vec{b}\right) + \vec{c} = \vec{a} + \left(\vec{b} + \vec{c}\right)$$ Associative property（結合法則）

$$\vec{a} + \vec{0} = \vec{a}$$ Existence of unique zero vector

$$\vec{a} + (-\vec{a}) = \vec{0}$$ Existence of unique inverse vector

Multiplication of scaler c :

$$c(\vec{a} + \vec{b}) = c\vec{b} + c\vec{a}$$

$$(c + d)\vec{a} = c\vec{a} + d\vec{a}$$

$$(cd)\vec{a} = c\,(d\vec{a})$$

$c \in \mathbb{R}$: Real vector space

$c \in \mathbb{C}$: Complex vector space

Inner product space (metric vector space)

（計量空間）

Inner product space:

Vector space + definition of inner product

Inner product: $(\vec{a}, \vec{b})$

Axiom:

$$(\vec{a}, \vec{a}) \geq 0$$

$$(\vec{a}, \vec{b}) = (\vec{b}, \vec{a})^*$$

$$(\vec{a} + \vec{b}, \vec{c}) = (\vec{a}, \vec{c}) + (\vec{b}, \vec{c})$$

$$(c\vec{a}, \vec{b}) = c(\vec{a}, \vec{b})$$

*If a norm defined from the inner product is "complete"（完備）,

that space is called **Hilbert space**.

Examples of vector spaces

(1) Coordinate space（数ベクトル空間） $\mathbb{R}^n, \mathbb{C}^n$

Vector: $$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad v_i \in \mathbb{R} \text{ or } \mathbb{C}$$

Inner product: $$(\vec{a}, \vec{b}) \equiv \vec{a} \cdot \vec{b}^*$$

(2) Wave vectors in quantum physics

Vector: $$|\Psi\rangle$$

Inner product: $$(|a\rangle, |b\rangle) = \langle b|a\rangle$$

Linearly independent or dependent
（線形独立） （線形従属）

Linear combination:

$$\vec{x} = c_1\vec{v}_1 + c_2\vec{v}_2 + \cdots c_k\vec{v}_k$$

$$\vec{v}_i \in \mathbb{V} \qquad c_i \in \mathbb{R} \text{ or } \mathbb{C}$$

A set $\{\vec{v}_1, \vec{v}_2, \cdots \vec{v}_k\}$ is **linearly independent** when

$\vec{x} = \vec{0}$ is satisfied if and only if $c_1 = c_2 = \cdots = c_k = 0$

$$\Updownarrow$$

A set $\{\vec{v}_1, \vec{v}_2, \cdots \vec{v}_k\}$ is **linearly dependent** when

it is not linearly independent.

Basis of vector space
（基底）

A set $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ $(\vec{e}_i \in \mathbb{V})$ is a basis（基底）of $\mathbb{V}$ when

$\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ is linearly independent.

and

Any vectors in $\mathbb{V}$ are represented by its linear combination.

$\vec{e}_i$: basis vector

# of basis vectors (n) is called **dimension** （次元）of $\mathbb{V}$.

$$n = \dim \mathbb{V}$$

Relation (map) to coordinate vector space

By using a basis $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$, $\vec{v} \in \mathbb{V}$ is uniquely represented as

(* From linear independency)

$$\vec{v} = v_1\vec{e}_1 + v_2\vec{e}_2 + \cdots v_n\vec{e}_n$$

➡ We can represent $\vec{v}$ as a coordinate vector

$$\vec{v} \rightarrow \begin{pmatrix} v_1 \\ v_2 \\ \cdots \\ v_n \end{pmatrix} \in \mathbb{C}^n(\text{ or } \mathbb{R}^n)$$

By selecting a basis, we obtain a "concrete" coordinate vector for an "abstract" vector

Orthonormal basis （正規直交基底）

When a vector space has an inner product,

$\vec{a}, \vec{b}$ is **orthogonal** （直交） if $(\vec{a}, \vec{b}) = 0$.

Orthonormal basis

A basis $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ is an orthonormal basis when

$$\|\vec{e}_i\| = 1 \qquad (i = 1, 2, \ldots, n)$$

$$(\vec{e}_i, \vec{e}_j) = 0 \qquad (i \neq j; i, j = 1, 2, \ldots, n)$$

*A basis can be transformed into an orthonormal basis.

cf. Gram-Schmidt orthonormalization

Example: quantum states

2 qbits:

We can choose the following four vectors as the (orthonormal) basis.

$$|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle$$

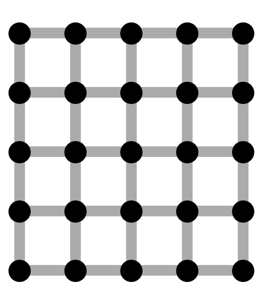
Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$$\Rightarrow \quad |\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta}|\alpha\beta\rangle$$

$C_{\alpha,\beta} = \langle\alpha\beta|\Psi\rangle$:complex number

$$C \in \mathbb{C}^4$$

Many qbits:



basis: $|m_1, m_2, \cdots, m_N\rangle = |00\cdots 0\rangle, |00\cdots 1\rangle, |01\cdots 0\rangle, \ldots$

$$|\Psi\rangle = \sum_{\{m_i=0,1\}} T_{m_1,m_2,\cdots,m_N}|m_1, m_2, \cdots, m_N\rangle$$

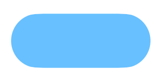
$$T_{m_1,m_2,\cdots,m_N} = \langle m_1, m_2, \cdots, m_N|\Psi\rangle \Rightarrow T \in \mathbb{C}^{2^N}$$

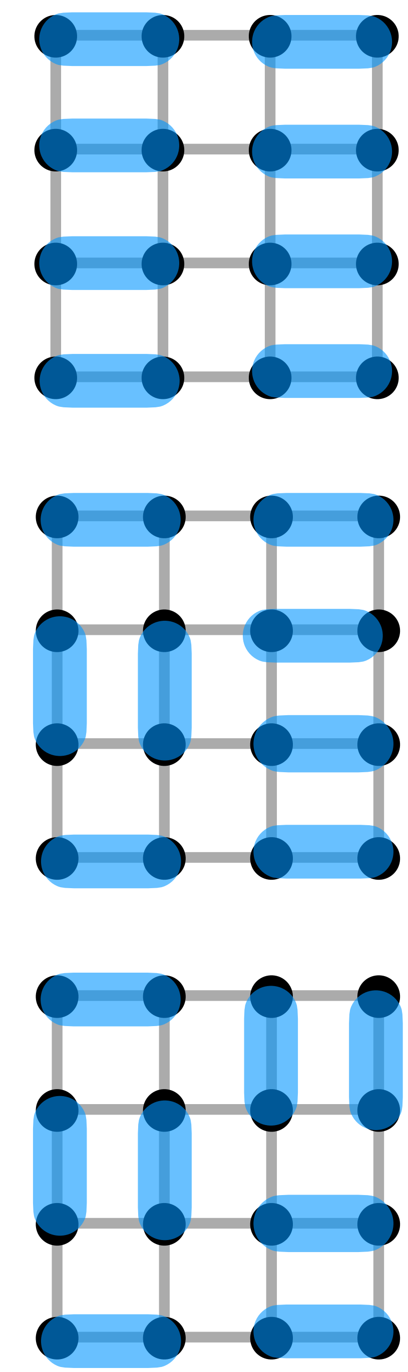
As an aside…

We may use unusual vector spaces in quantum many-body problems.

Quantum dimer model

(D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1988))

“Dimer”  $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

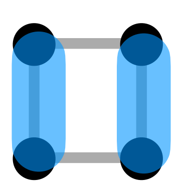
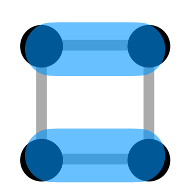


Orthonormal basis: All closed packing of dimers

(When we use the usual S=1/2 spins, they are not orthogonal.)

$$\mathcal{H} = \sum_{\text{plaquettes}} \Big[\underbrace{-J\left(|\,||\rangle\langle = | + \text{H.C.}\right)}_{\text{Flip of a dimer pair}} + V \underbrace{\left(|\,||\rangle\langle || \,| + | = \rangle\langle = |\right)}_{\text{Potential energy}} \Big]$$

States of a plaquette

$|\,||\rangle$ =  $| = \rangle$ = 

Vector subspace (linear subspace)

Vector subspace（ベクトル部分空間）**:**

A subset $\mathbb{W}$ of a vector space $\mathbb{V}$ is a vector subspace of $\mathbb{V}$ when $\mathbb{W}$ satisfies the same axioms of vector space with $\mathbb{V}$.

The following conditions are necessary and sufficient.

$$\vec{a}, \vec{b} \in \mathbb{W} \Rightarrow \vec{a} + \vec{b} \in \mathbb{W}$$

$$\vec{a} \in \mathbb{W}, c \in \mathbb{C} \Rightarrow c\vec{a} \in \mathbb{W}$$

(In the case of complex vector space)

*The dimension of a vector subspace can be smaller than that of the original vector space.

$\Rightarrow$ If we construct an efficient vector subspace, it can be a kind of data compression.

Matrix and linear map

Matrix（行列）

Matrix: "Table" of (complex) numbers in a rectangular form

$M \times N$ matrix

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & \cdots & A_{2,N} \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{M,N} \end{pmatrix}$$

$$A_{ij} \in \mathbb{C}(\text{ or } \mathbb{R})$$

Product of matrices: $C = AB$

$$A : M \times K$$
$$B : K \times N$$
$$C : M \times N$$

$$C_{ij} = \sum_{k=1}^{K} A_{ik} B_{kj}$$

In general: $XY \neq YX$

*We also know addition, multiplication of scalar.

Identity matrix（単位行列）

Identity matrix:

$N \times N$ matrix
(Square matrix)

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

Product:

$$IA = A \qquad A : N \times M$$

$$BI = B \qquad B : K \times N$$

* Element of the identity matrix: $I_{ij} = \delta_{ij}$ (Kronecker delta)

$$\delta_{ij} = \begin{cases} 1 & (i = j) \\ 0 & (i \neq j) \end{cases}$$

Transpose, complex conjugate and adjoint

Transpose:
(転置)

$$A^t \qquad (A^t)_{ij} = A_{ji}$$

Complex conjugate:
(複素共役)

$$A^* \qquad (A^*)_{ij} = A^*_{ij}$$

Adjoint:
(随伴)

or

Hermitian conjugate:
(エルミート共役)

$$A^\dagger = (A^t)^* = (A^*)^t$$

$$(A^\dagger)_{ij} = A^*_{ji}$$

("Dagger" is convention in physics)

Multiplication to coordinate vector

$$A : M \times N \qquad \vec{v} \in \mathbb{C}^N \qquad \vec{v}' \in \mathbb{C}^M$$

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & \cdots & A_{2,N} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{M,N} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} v'_1 \\ v'_2 \\ \vdots \\ \vdots \\ v'_M \end{pmatrix}$$

M × *N* matrix transforms an *N*-dimensional coordinate vector to an *M*-dimensional coordinate vector.

M × N matrix $\xleftrightarrow[\text{1 to 1}]{}$ **Linear map:** $\mathbb{C}^N \to \mathbb{C}^M$

（線形写像）

General linear map

Map: $f : \mathbb{V} \to \mathbb{V}'$

$$f(\vec{v}) = \vec{v}' \qquad (\vec{v} \in \mathbb{V}, \vec{v}' \in \mathbb{V}')$$

Linear map:

$$f(\vec{x} + \vec{y}) = f(\vec{x}) + f(\vec{y})$$

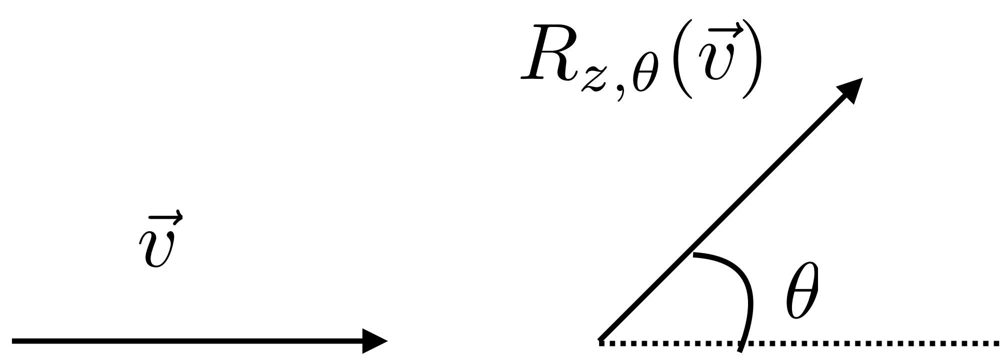
$$f(c\vec{x}) = cf(\vec{x})$$

$$(\vec{x}, \vec{y} \in \mathbb{V}, c \in \mathbb{C})$$

Examples:

Rotation (e.g. θ rotation around z-axis)

$$R_{z,\theta} : \mathbb{C}^3 \to \mathbb{C}^3$$



Hamiltonian operator

$$\mathcal{H} : \mathbb{V} \to \mathbb{V}$$

$$|\Psi\rangle \Rightarrow \mathcal{H}|\Psi\rangle$$

Matrix representation of linear map

By using a basis, we can represent a linear map in a matrix.

$$f : \mathbb{V} \to \mathbb{V}'$$

Vector space $\mathbb{V} : \dim \mathbb{V} = N$ → $\mathbb{V}' : \dim \mathbb{V}' = M$

Basis $\{\vec{e}_1, \vec{e}_2, \cdots, \vec{e}_N\}$ → $\{\vec{e'}_1, \vec{e'}_2, \cdots, \vec{e'}_M\}$

Transformation of basis vectors:

$$f(\vec{e}_j) = f_{1j}\vec{e'}_1 + f_{2j}\vec{e'}_2 + \cdots + f_{Mj}\vec{e'}_M$$

* For orthonormal basis, $f_{ij} = (f(\vec{e}_j), \vec{e'}_i)$

→ $f : \mathbb{V} \to \mathbb{V}'$ ↔ **1 to 1** (if we fix basis)

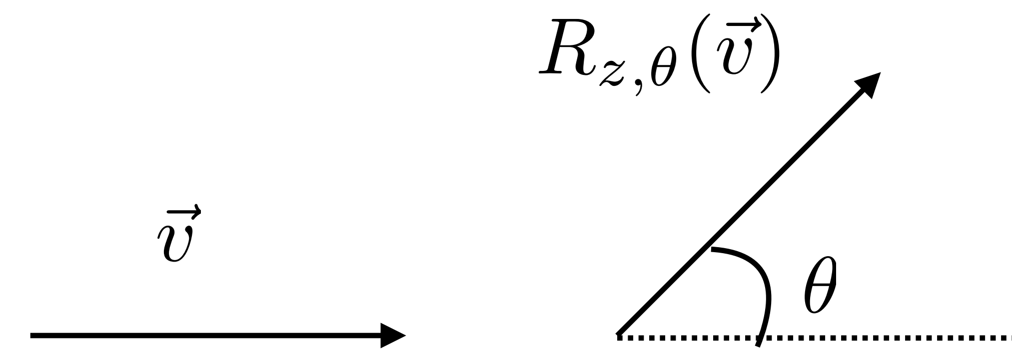
$$\begin{pmatrix} f_{11} & f_{12} & \cdots & f_{1,N} \\ f_{21} & f_{22} & \cdots & f_{2,N} \\ \vdots & \vdots & & \vdots \\ f_{M1} & f_{M2} & \cdots & f_{M,N} \end{pmatrix}$$

Examples of matrix

Rotation (e.g. θ rotation around z-axis)

$$R_{z,\theta} : \mathbb{C}^3 \to \mathbb{C}^3$$

$$R_{z,\theta} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



Hamiltonian operator

$$\mathcal{H} : \mathbb{V} \to \mathbb{V}$$

$$\mathcal{H} \to \begin{pmatrix} H_{0,0;0,0} & H_{0,0;0,1} & H_{0,0;1,0} & H_{0,0;1,1} \\ H_{0,1;0,0} & H_{0,1;0,1} & H_{0,1;1,0} & H_{0,1;1,1} \\ H_{1,0;0,0} & H_{1,0;0,1} & H_{1,0;1,0} & H_{1,0;1,1} \\ H_{1,1;0,0} & H_{1,1;0,1} & H_{1,1;1,0} & H_{1,1;1,1} \end{pmatrix}$$

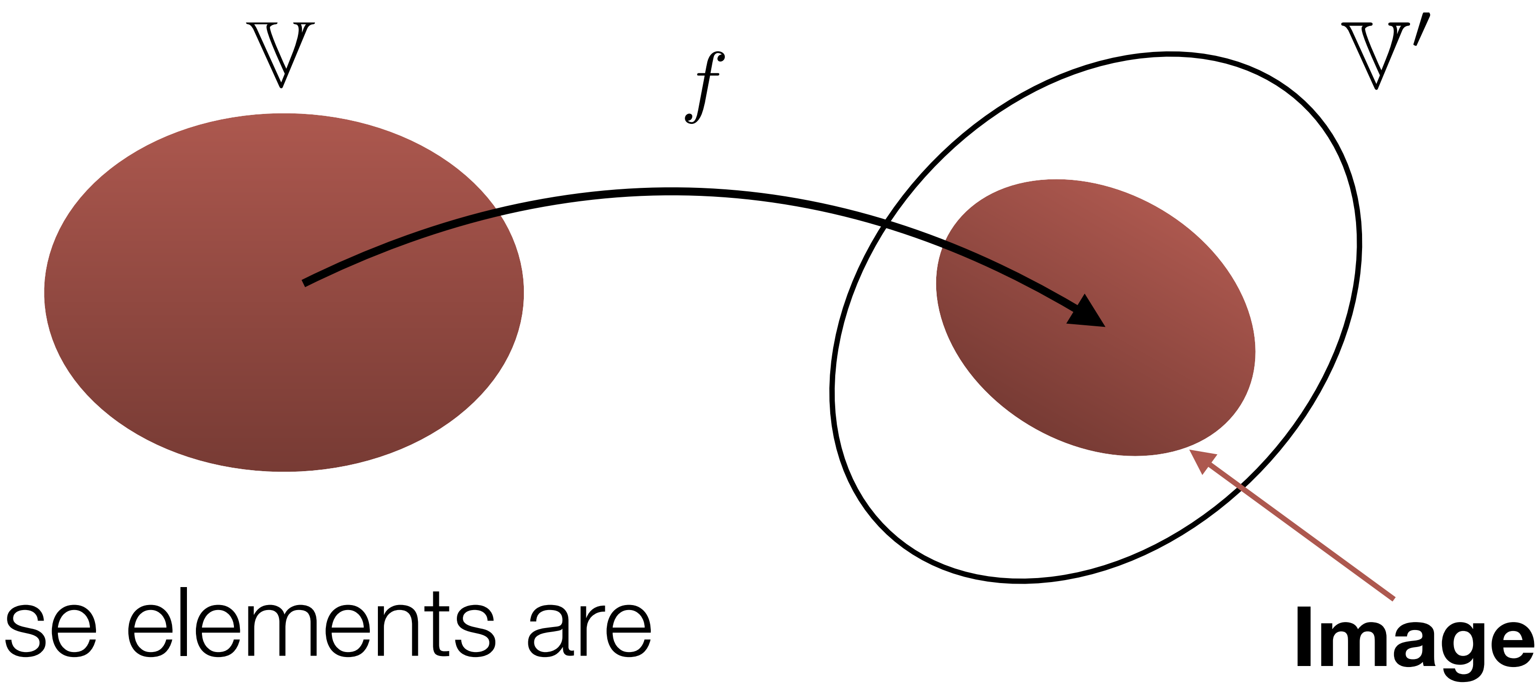
Matrix element: $H_{\alpha,\beta;\alpha',\beta'} \equiv \langle \alpha\beta | \mathcal{H} | \alpha'\beta' \rangle$
（行列要素）

* In this notation, basis should be orthonormal.

Image of a map

$f : \mathbb{V} \to \mathbb{V}'$

Image of f:
(像)



Vector subspace whose elements are mapped from $\mathbb{V}$ by f.

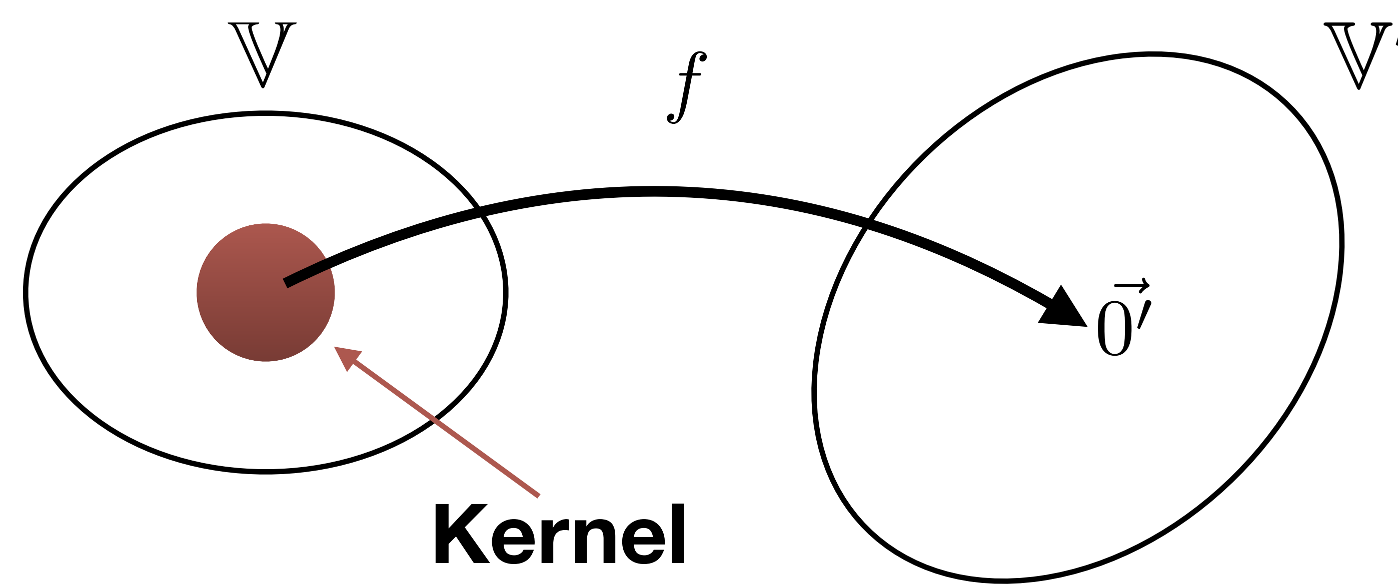
$$\mathrm{img}(f) = \{\vec{v}' | \vec{v} \in \mathbb{V}, \vec{v}' = f(\vec{v})\}$$

Kernel of a map

$f : \mathbb{V} \to \mathbb{V}'$

Kernel of f:

(核)



Vector subspace whose elements are mapped into zero vector by f .

$$\ker(f) = \{\vec{v} | \vec{v} \in \mathbb{V}, f(\vec{v}) = \vec{0}'\}$$

Theorem:

$$\dim(V) = \dim(\ker(f)) + \dim(\mathrm{img}(f))$$

Rank of matrix

Rank （ランク or 階数）of a matrix *A*:

$$\mathrm{rank}(A) \equiv \dim(\mathrm{img}(A))$$

Rank is identical with

Maximum # of linearly independent column vectors （列ベクトル）in *A*

Maximum # of linearly independent row vectors （行ベクトル）in *A*

$$\mathrm{rank}(A) \leq \min(M, N)$$

for an *M*×*N* matrix *A*.

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & \cdots & A_{2,N} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{M,N} \end{pmatrix}$$

Regular matrix and its inverse matrix

A square matrix A is a **regular matrix** （正則）if a matrix X satisfying

$$AX = XA = I$$

exists. The matrix X is called inverse matrix（逆行列） of A and it is written as $X = A^{-1}$.

Properties: A^{-1} is unique.

$$(A^{-1})^{-1} = A$$

$$(AB)^{-1} = B^{-1}A^{-1}$$

A is a regular matrix $\Longleftrightarrow$ $\mathrm{rank}(A) = N$

Can we consider an "inverse matrix" of a non-regular matrix (including a rectangular matrix) ?

Simultaneous linear equation

Simultaneous linear equation（連立一次方程式）

can be represented by a matrix and a vector as

$$A\vec{x} = \vec{b} \qquad\qquad A : M \times N, \vec{x} \in \mathbb{C}^N, \vec{b} \in \mathbb{C}^M$$

If A is a square matrix (*N*=*M*), and it has an inverse matrix (rank(*A*) =N), we can solve the equation as

$$\vec{x} = A^{-1}\vec{b}$$

N > *M*: Underdetermined problem （劣決定問題）

N < *M*: Overdetermined problem （優決定問題）

How can we find a "solution" when A does not have the "inverse"?

→ It is related to "sparse modeling".

(Although we will not treat it, it is a kind of data compression)

Eigenvalue problems and diagonalization

Eigenvalue and Eigenvector

For a square matrix A

$$A\vec{v} = \lambda\vec{v}$$

$\vec{v} \neq \vec{0}$:eigenvector（固有ベクトル）

$\lambda \in \mathbb{C}$:eigenvalue（固有値）

Properties:

If $\vec{v}$ is an eigenvector, $c\vec{v}$ is also an eigenvector.

Eigenspace（固有空間）：

The set of eigenvectors corresponds an eigenvalue λ.

Eigenvectors corresponding to different eigenvalues are linearly independent.

Example: quantum many-body problems

$\boxed{\text{Schrödinger equation}}$

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

$\mathcal{H}$:Hamiltonian

$|\Psi\rangle$:Wave function (state vector)

E :Energy

Eigenvalue = energy

Eigenvector = quantum state (eigenstate)

Typical questions:

- How does the lowest energy vary when we change the Hamiltonian?
  - What is the energy gap between the lowest and the 2nd lowest states?
- What is the property of the eigenstate?
  - Quantum phase transitions

Right and left eigenvectors

In general, left eigenvectors can be different from the right eigenvectors.

$$A\vec{v} = \lambda\vec{v}$$

$$(\vec{u}^*)^t A = \lambda(\vec{u}^*)^t$$

Cf. $|\psi\rangle, \langle\phi|$ in quantum state

$\vec{v}$:Right eigenvector

$(\vec{u}^*)^t$:Left eigenvector

Properties:

The set of eigenvalues is identical between the right and the left eigenvectors.

A left eigenvector and a right eigenvector are orthogonal when they correspond to different eigenvalues.

$$\vec{u}_i^* \cdot \vec{v}_j = 0 \qquad (\lambda_i \neq \lambda_j)$$

Diagonalization

Diagonalizaiton（対角化）：

$$A : N \times N$$

$$P^{-1}AP = \begin{pmatrix} \alpha_1 & & & \\ & \alpha_2 & & \\ & & \ddots & \\ & & & \alpha_N \end{pmatrix}$$

A can be diagonalized. ⟺ *A* has *N* linearly independent eigenvectors.

necessary and sufficient

$$\alpha_i = \lambda_i$$

$$P = (\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_N)$$

$$(P^{-1})^t = (\vec{u}_1^*, \vec{u}_2^*, \cdots, \vec{u}_N^*)$$

Normalization: $\vec{u}_i^* \cdot \vec{v}_i = 1$

Unitary matrix

Unitary matrix（ユニタリ行列）： $U^\dagger = U^{-1}$

Real Orthogonal matrix（実直交行列）： $P^t = P^{-1}, (P_{ij} \in \mathbb{R})$

When we consider a unitary matrix as a set of vectors:

$$U = (\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_N)$$

it is a orthonormal basis: $\vec{v}_i^* \cdot \vec{v}_j = \delta_{i,j}$

The linear map represented by a unitary matrix (**unitary transformation**) does not change

- the norm of a vector

$$\|U\vec{v}\| = \|\vec{v}\|$$

- "distance" between two vectors

$$\|U\vec{v}_1 - U\vec{v}_2\| = \|\vec{v}_1 - \vec{v}_2\|$$

Normal matrix

Normal matrix（正規行列）： $A^\dagger A = AA^\dagger$

We can always diagonalize it by a unitary matrix

$$U^\dagger = U^{-1}$$

as

$$U^\dagger A U = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix} \qquad \lambda_i \in \mathbb{C}$$

Its eigenvalues could be complex.

(even if *A* is a real matrix)

Hermitian matrix and its eigenvalue

Hermitian matrix（エルミート行列）：$A^\dagger = A$

Real symmetric matrix（実対称行列）： $A^t = A, \quad (A_{ij} \in \mathbb{R})$

It is a special normal matrix. $A^\dagger A = AA^\dagger = AA$

Its eigenvalues are real.

We can always diagonalize it by a unitary matrix

$$U^\dagger A U = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix} \qquad \lambda_i \in \mathbb{R}$$

Hermitian (or real symmetric) matrices often appear in physics.

Ex. Hamiltonian, $\mathcal{H}$

Generalization of diagonalization

- Eigenvalue problems and diagonalizations are defined for a square matrix.
- Even if A is a square matrix, it may not be diagonalized.

- Is it possible to transform all square matrixes into diagonal forms by generalizing the diagonalization?
- Is it possible to generalize it to a rectangular matrices?

Yes. **The singular value decomposition** (特異値分解) is an generalization of the diagonalization.

(We can also consider a decomposition of a tensor.)

Next week (Oct. 20)

Notice

- No classes on Nov. 3, Nov. 17, and Nov. 22
- Classes will be also held on Jan. 5 and Jan. 19

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1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network