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

理学系研究科 大久保 毅

Graduate School of Science, Tsuyoshi Okubo

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**

 $|\Psi
angle$

Geometric vector

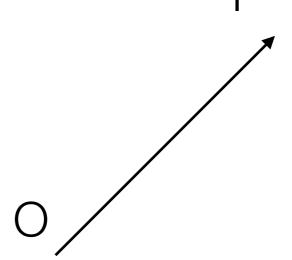
Geometric vector: Arrow on the plane (or the space),

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:

$$(\vec{a}, \vec{b}) \equiv \vec{a} \cdot \vec{b}$$
$$= a_x b_x + a_y b_y + a_z b_z$$

Properties:

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

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

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

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

$$c \in \mathbb{R}$$

Norm (length):

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

Example:

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

Vector space (linear space)

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

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

Properties of addition:

$$\vec{a} + \vec{b} = \vec{b} + \vec{a}$$

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

$$\vec{a} + \vec{0} = \vec{a}$$

$$\vec{a} + (-\vec{a}) = \vec{0}$$

Multiplication of scaler $\,c\,$:

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

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

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

Commutative property (交換法則)

Associative property (結合法則)

Existence of unique zero vector

Existence of unique inverse vector

 $c \in \mathbb{R}$: 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:

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

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

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

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

*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) $\mathbb{R}^n, \mathbb{C}^n$

$$ec{v} = egin{pmatrix} v_1 \ v_2 \ dots \ v_n \end{pmatrix} \qquad v_i \in \mathbb{R} \ ext{or} \ \mathbb{C}$$

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 $c_1 = c_2 = \cdots = c_k = 0$



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.

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



 \vec{e}_i : basis vector

and

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 $\vec{v}=v_1\vec{e}_1+v_2\vec{e}_2+\cdots v_n\vec{e}_n$ (* From linear independency)



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

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

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

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

*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: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

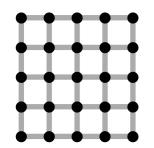


$$|\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta} |\alpha\beta\rangle$$

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

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

Many qbits:



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

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

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

We may consider a different orthonormal basis for 2-qubit states.

Bell basis
$$|\Phi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle \pm |11\rangle\right)$$
 $|\Psi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle \pm |10\rangle\right)$

*These are *maximally* entangled states.

Basis 1 (computational basis)

$$\vec{e}_1 = |00\rangle$$

$$\vec{e}_2 = |01\rangle$$

$$\vec{e}_3 = |10\rangle$$

$$\vec{e}_4 = |11\rangle$$

$$|00\rangle \rightarrow \begin{pmatrix} 1\\0\\0\\0\\0 \end{pmatrix}$$

Basis 2 (Bell basis)

$$\vec{e}_1 = |00\rangle$$

$$\vec{e}_2 = |01\rangle$$

$$\vec{e}_3 = |10\rangle$$

$$\vec{e}_4 = |11\rangle$$

$$|00\rangle \rightarrow \begin{pmatrix} 1\\0\\0\\0\\0 \end{pmatrix}$$

$$\vec{e}_1 = |\Phi^+\rangle$$

$$\vec{e}_2 = |\Phi^-\rangle$$

$$\vec{e}_3 = |\Psi^+\rangle$$

$$\vec{e}_4 = |\Psi^-\rangle$$

$$|00\rangle \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1\\0\\0 \end{pmatrix}$$

When we change the basis, the corresponding coordinate vector changes.

As an aside...

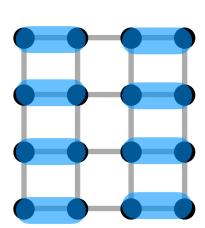
We may use unusual vector spaces in quantum many-body problems.

Quantum dimer model

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



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





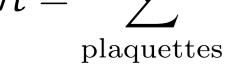
Orthonormal basis: All closed packing of dimers

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

$$\mathcal{H} = \sum \left[-J(|\parallel\rangle\langle=|+\text{H.C.}) + V(|\parallel\rangle\langle\|\mid+|=\rangle\langle=|) \right]$$

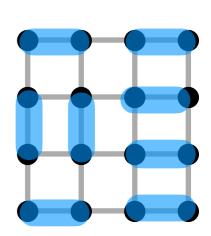
Flip of a dimer pair

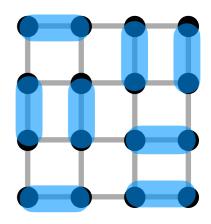
Potential energy



States of a plaquette

$$| = \rangle =$$





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.

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

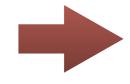
$$\vec{a} + \vec{b} \in \mathbb{W}$$

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

$$\vec{c}\vec{a} \in \mathbb{W}$$

(In the case of complex vector space)

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



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

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

Product of matrices: C = AB

$$C_{ij} = \sum_{k=0}^{K} A_{ik} B_{kj}$$

$$A: M \times K$$

$$B: K \times N$$

$$C: M \times N$$

In general: $XY \neq YX$

*We also know addition, multiplication of scalar.

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

Identity matrix (単位行列)

Identity matrix:

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

Product:

$$IA = A$$

$$A: N \times M$$

$$BI = B$$

* 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: A^* $(A^*)_{ij} = A^*_{ij}$ (複素共役)

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

Adjoint: (随伴)

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

or

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

Hermitian conjugate:

(エルミート共役)

("Dagger" is convention in physics)

Multiplication to coordinate vector

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

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

 $M \times N$ matrix transforms an N-dimensional coordinate vector to an M-dimensional coordinate vector.



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:

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

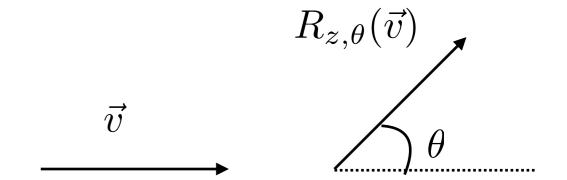
$$f(c\vec{x}) = cf(\vec{x})$$

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

Examples:

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

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



Hamiltonian operator

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



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

$$\mathbb{V}: \dim \mathbb{V} = N$$

Basis

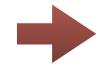
$$\{\vec{e}_1,\vec{e}_2,\cdots,\vec{e}_N\}$$



$$\mathbb{V}' : \dim \mathbb{V}' = M$$
$$\{\vec{e'}_1, \vec{e'}_2, \cdots, \vec{e'}_M\}$$

Transformation of basis vectors:

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



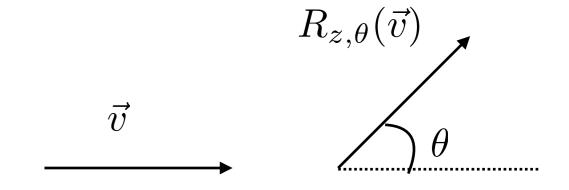
$$f: \mathbb{V} \to \mathbb{V}'$$

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

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

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

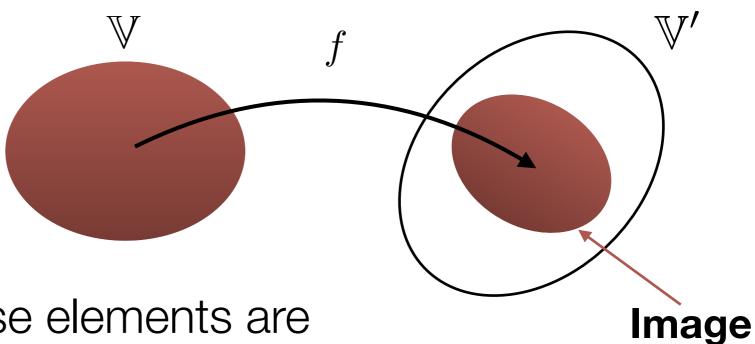
* In this notation, basis should be orthonormal.

Image of a map

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

Image of f:

(像)



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

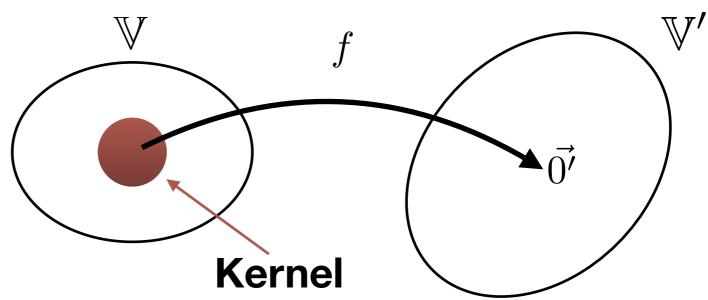
$$\operatorname{img}(f) = \{ \vec{v}' | \vec{v} \in \mathbb{V}, \vec{v}' = f(\vec{v}) \}$$

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:

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

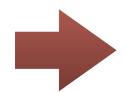
Rank of matrix

Rank (ランク or 階数)of a matrix A:

$$rank(A) \equiv \dim(img(A))$$

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*



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

for an $M \times N$ matrix A.

A_{11}	A_{12}	• • •	$A_{1,N}$
A_{21}	A_{22}		$A_{2,N}$
	•		:
	•		•
	•		:
A_{M1}	A_{M2}	• • •	$A_{M,N}$

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 $\operatorname{rank}(A) = N$



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

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

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)

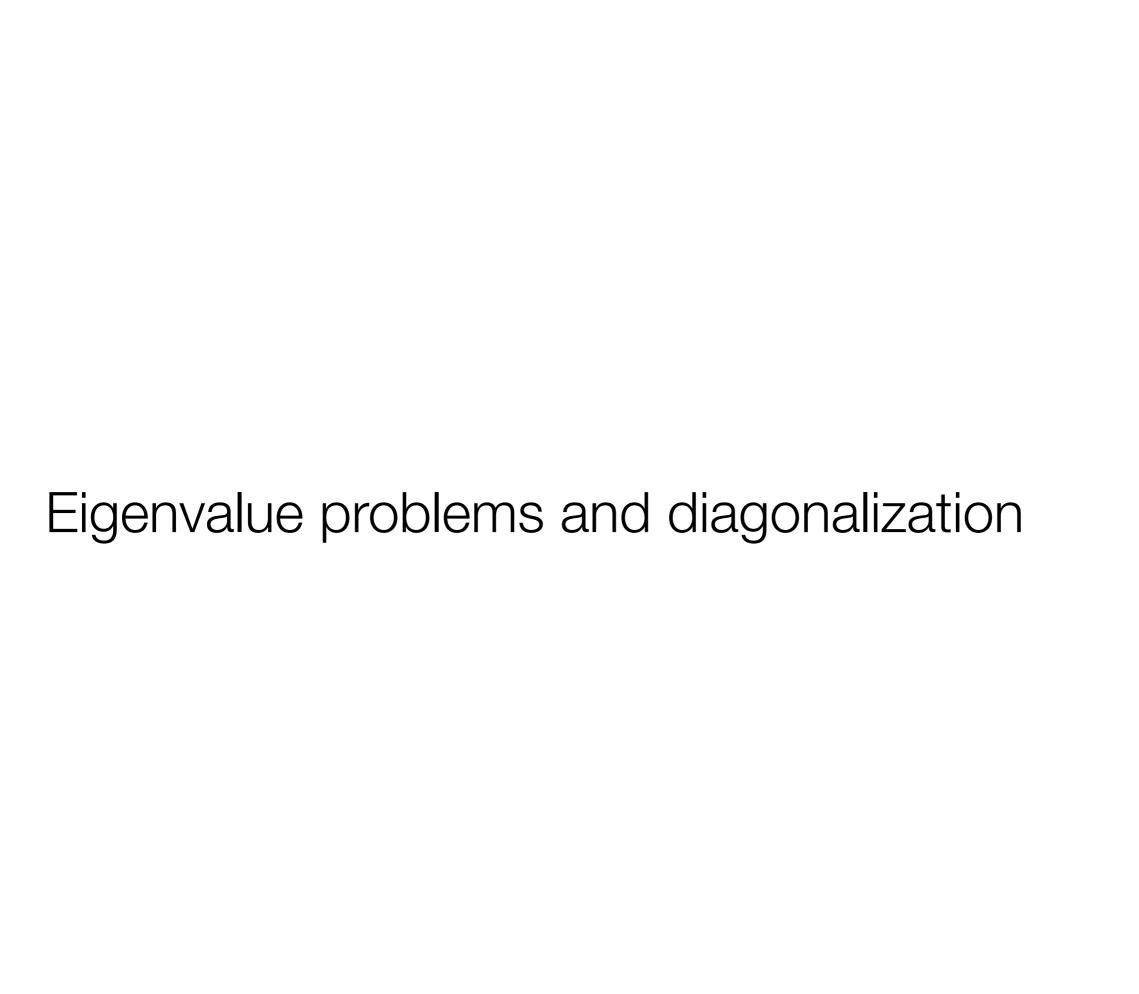
N < M: Overdetermined problem (優決定問題)

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 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

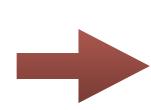
Schrödinger equation

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

 ${\cal H}$:Hamiltonian

 $|\Psi
angle$: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.

$$Aec{v}=\lambdaec{v}$$
 $_{ ext{Cf. }|\psi
angle,\langle\phi|}$ $(ec{u}^*)^tA=\lambda(ec{u}^*)^t$ 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.

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

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.

$$\alpha_{i} = \lambda_{i}$$

$$P = (\vec{v}_{1}, \vec{v}_{2}, \cdots, \vec{v}_{N})$$

$$(P^{-1})^{t} = (\vec{u}_{1}^{*}, \vec{u}_{2}^{*}, \cdots, \vec{u}_{N}^{*})$$

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

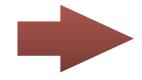
- the norm of a vector $\|U\vec{v}\| = \|\vec{v}\|$
- "distance" between two vectors

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



Normal matrix

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



We can always diagonalize it by a unitary matrix

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

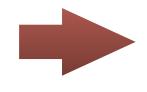
as
$$U^\dagger A U = egin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \lambda_N \end{pmatrix} \qquad \lambda_i \in \mathbb{C}$$

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

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

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

(特異值分解) is an generalization of the diagonalization.

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

Notice

Next week (Oct. 20)

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