計算科学における情報圧縮

Information Compression in Computational Science 2021.12.16

#10:高度なデータ圧縮:情報のエンタングルメントと行列積表現

Entanglement of information and matrix product states

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Schedule

1st: Huge data in modern physics (Today)

2nd: Information compression in modern physics

(+review of linear algebra)

3rd: Review of linear algebra (+ singular value decomposition)

4th: Singular value decomposition and low rank approximation

5th: Basics of sparse modeling

6th: Basics of Krylov subspace methods

7th: Information compression in materials science

8th: Accelerating data analysis: Application of sparse modeling

9th: Data compression: Application of Krylov subspace method

10th: Entanglement of information and matrix product states

11th: Matrix product states + Application of MPS to eigenvalue problems

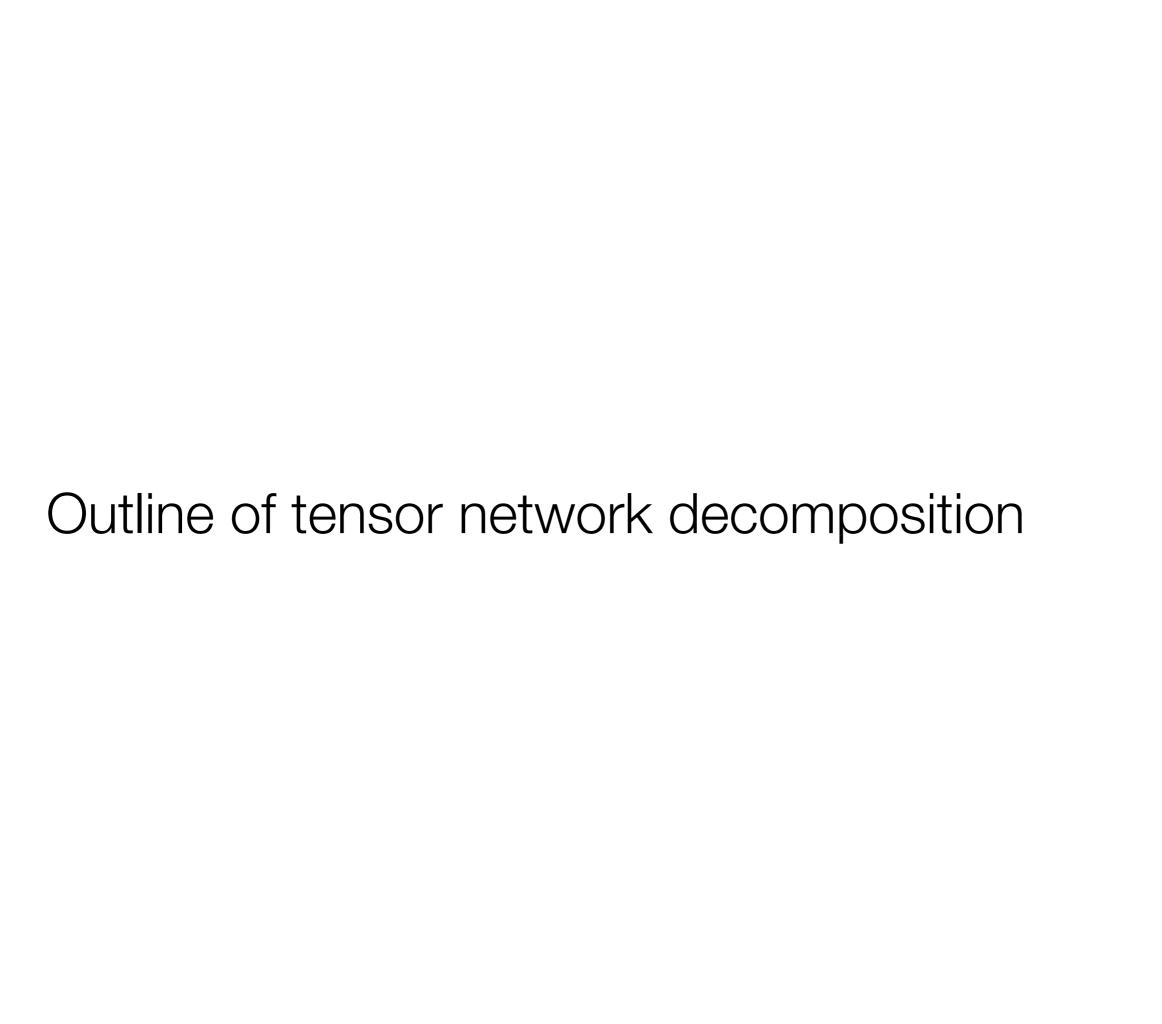
12th: Application of MPS to time evolution and data science

13th: Other tensor network representations

+ (Appendix: Information compression by tensor network renormalization)

Outline

- Outline of tensor network decomposition
- Entanglement
 - Schmidt decomposition
 - Entanglement entropy and its area law
- Matrix product states
 - Matrix product states (MPS)
 - Canonical form
 - infinite MPS



Classification of Information Compression by Memory Costs

Linear algebra for huge data: $\vec{v} \in \mathbb{C}^M$

- (1) A matrix can be stored Required memory~ $O(M^2)$
- (2) Although a matrix cannot be stored, vectors can be stored Required memory $\sim O(M)$
- (3) A vector cannot be stored

Required memory $\ll O(M)$

We try to approximate a vector in a compact form.

$$M \sim a^N$$
 Memory ~ $O(N^x)$

Exponential

Polynomial

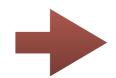
N:problem size (e.g. system size)

When we efficiently compress a vector?

$$\vec{v} = \sum_{i=1}^{M} C_i \vec{e_i} \qquad \vec{v} \in \mathbb{C}^M$$

If we can find a basis where the coefficients have a structure (correlation).

(1) Almost all C_i are zero (or very small).



We store only a few finite elements $\{(i,C_i)\}$

E.g. Fourier transformation
$$\vec{v} = \sum_{k=1}^{M} D_k \vec{f}_k$$

If we can neglect larger wave numbers, we can efficiently approximate the vector with smaller number of coefficients.

Classical state
$$|\Psi\rangle=|01011\dots00\rangle$$

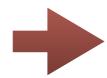
In this case, we know that only a specific C_i is non-zero.

We need only an integer corresponding to the non-zero element.

When we efficiently compress a vector?

$$\vec{v} = \sum_{i=1}^{M} C_i \vec{e}_i \qquad \vec{v} \in \mathbb{C}^M$$

(2) All of C_i are not necessarily independent.



We store "structure" and "independent elements".

$$\{(i,C_i)\}$$

E.g. Product state ("generalized" classical state)

A vector is decomposed into product of small vectors.

$$|\Psi
angle=|\phi_1
angle\otimes|\phi_2
angle\otimes\cdots$$
 e.g. (It is identical to the rank-1 CP decomposition.) $|\phi_1
angle=\alpha|0
angle+\beta|1
angle$ $|\phi_1
angle=|01
angle-|10
angle$

structure: "product state"

independent elements: small vectors

Tensor network decomposition of a vector

Target:

Exponentially large

Hilbert space

$$\vec{v} \in \mathbb{C}^M$$
 with $M \sim a^N$

Total Hilbert space is decomposed as a product of "local" Hilbert space.

$$\mathbb{C}^M = \mathbb{C}^a \otimes \mathbb{C}^a \otimes \cdots \mathbb{C}^a$$

*Local Hilbert space dimensions can be different.

Examples:

Picture image:

256 × 256 pixel image → 216 dimensional vector

 \rightarrow 16-leg tensor (with a = 2)

Probability distribution:

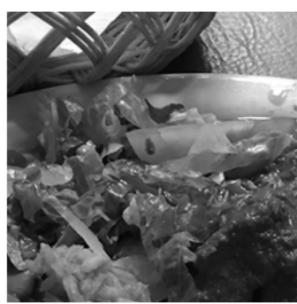
e.g. Ising model
$$P(\{S_i\}) = \frac{e^{\beta J \sum_{\langle i,j \rangle} S_i S_j}}{Z}$$

 \rightarrow 2^N vector \rightarrow N-leg tensor (with a=2)

Wave function:

$$|\Psi\rangle = \sum_{\{m_i=0,1\}} T_{m_1,m_2,\cdots,m_N} | m_1,m_2,\cdots,m_N \rangle \rightarrow T_{m_1,m_2,\cdots,m_N} : N$$
-leg tensor

256=**2**8

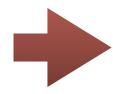


Tensor network decomposition of a vector

Target:

Exponentially large Hilbert space

$$\vec{v} \in \mathbb{C}^M \qquad \mathbb{C}^M = \mathbb{C}^a \otimes \mathbb{C}^a \otimes \cdots \mathbb{C}^a$$

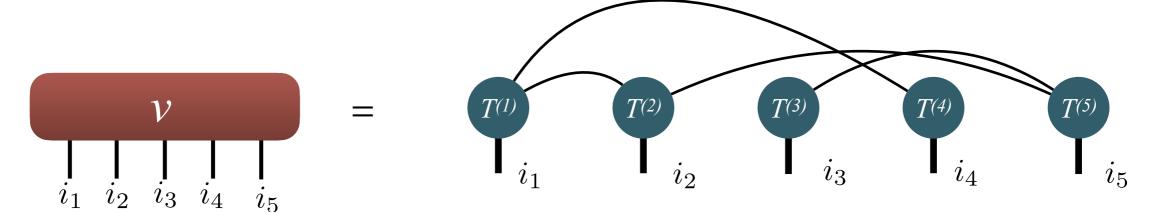


Tensor network decomposition

$$v_i = v_{i_1, i_2, \dots, i_N} = \sum_{\{x\}} T^{(1)}[i_1]_{x_1, x_2, \dots} T^{(2)}[i_2]_{x_1, x_3, \dots} \cdots T^{(N)}[i_N]_{x_3, x_{100}, \dots}$$

 $i_n = 0, 1, \dots, a-1$: index of local Hilbert space

$$T[i]_{x_1,x_2,...}$$
: local tensor for "state" i



Graphical representations for tensor network

Vector

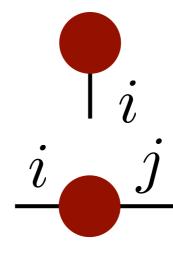
$$ec{v}:v_i$$



$$M$$
 : $M_{i,j}$

Tensor

$$T:T_{i,j,k}$$



$$\frac{i}{k}$$

* n-rank tensor = n-leg object

When indices are not presented in a graph, it represent a tensor itself.

Graphical representations for tensor network

Matrix product

$$C_{i,j} = (AB)_{i,j} = \sum_{k} A_{i,k} B_{k,j}$$

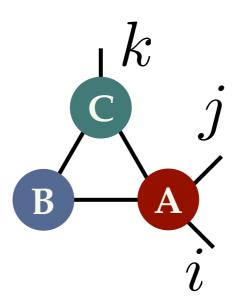
$$C = AB$$

$$\frac{i}{\mathbf{C}} = \frac{i}{\mathbf{A}} \frac{k}{\mathbf{B}} \frac{j}{j}$$

$$-C-=-A-B-$$

Generalization to tensors

$$\sum_{\alpha,\beta,\gamma} A_{i,j,\alpha,\beta} B_{\beta,\gamma} C_{\gamma,k,\alpha}$$

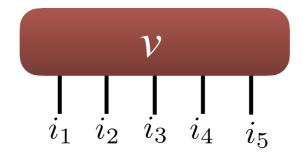


Contraction of a network = Calculation of a lot of multiplications (縮約)

Diagram for a tensor network decomposition

Vector

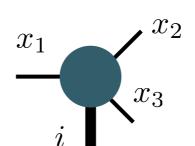
$$v_{i_1,i_2,i_3,i_4,i_5}$$



*Vector looks like a tensor

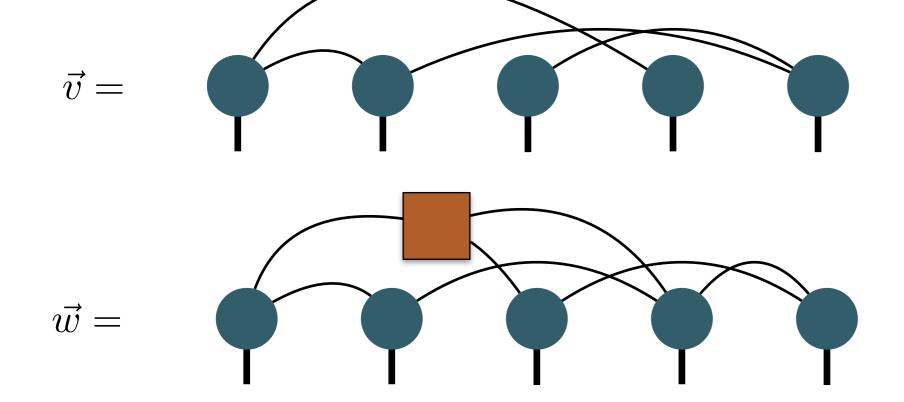
Tensor

$$T[i]_{x_1, x_2, x_3}$$



*We treat *i* as an index of the tensor.

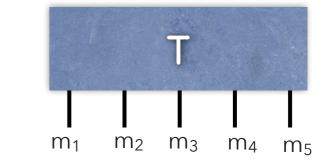
Tensor network decomposition



*We can consider tensors independent on i.

Another "generalization" of SVD to tensors.

 T_{m_1,m_2,\cdots,m_N} :N-leg tensor (or Vector)

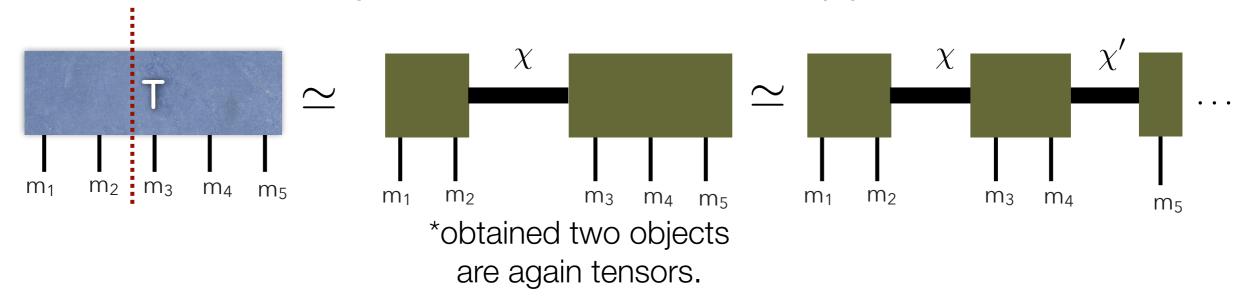


Cf. wave function:
$$|\Psi\rangle=\sum_{\{m_i=0,1\}}T_{m_1,m_2,\cdots,m_N}|m_1,m_2,\cdots,m_N\rangle$$

We can consider it as a matrix by making two groups:

$$T_{\{m_1, m_2, \cdots, m_M\}, \{m_{M+1}, \cdots, m_N\}}$$

We can perform the low rank approximation of T.



What does it mean?



It is related to MPS

Entanglement (エンタングルメント)

N-qubit system (S=1/2 quantum spin system)

Example vector: Wave function of N-qubit systems

$$\begin{aligned} |\Psi\rangle &= \sum_{\{i_1,i_2,\dots i_N\}} \Psi_{i_1i_2\dots i_N} |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle \\ &= \sum_{\{i_1,i_2,\dots i_N\}} \Psi_{i_1i_2\dots i_N} |i_1i_2\dots i_N\rangle \end{aligned}$$

Coefficients = vector: $\vec{\Psi} \in \mathbb{C}^{2^N}$

* Inner product: $\langle \Phi | \Psi \rangle = \vec{\Phi}^* \cdot \vec{\Psi}$

Schmidt decomposition

General vector:
$$\vec{x} \in \mathbb{V}_1 \otimes \mathbb{V}_2$$
 dim $\mathbb{V}_1 = n_1$, dim $\mathbb{V}_2 = n_2$

$$\dim \mathbb{V}_1 = n_1, \dim \mathbb{V}_2 = n_2$$
$$(n_1 \ge n_2)$$

Schmidt decomposition

There exists special basis which satisfies

$$ec{x} = \sum_{i=1}^{n_2} \lambda_i ec{u}_i \otimes ec{v}_i$$
 No off-diagonal coupling!

Orthonormal basis

$$\{\vec{u}_1, \vec{u}_2, \dots, \vec{u}_{n_1}\} \in \mathbb{V}_1$$

 $\{\vec{v}_1, \vec{v}_2, \dots, \vec{v}_{n_2}\} \in \mathbb{V}_2$

Schmidt coefficient $\lambda_i > 0$

Schmidt decomposition is unique.

Schmidt decomposition for a wave function

Wave function:
$$|\Psi\rangle = \sum_{\{i_1,i_2,...i_N\}} \Psi_{i_1i_2...i_N} |i_1i_2...i_N\rangle$$

Schmidt decomposition

Divide a system into two parts, A and B:





General wave function can be represented by a superposition of orthonormal basis set.

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle = \sum_i \lambda_i |\alpha_i\rangle \otimes |\beta_i\rangle$$

$$M_{i,j} \equiv \Psi_{(i_1,\dots),(\dots,i_N)} \quad |A_i\rangle = |i_1,i_2,\dots\rangle$$

$$A \quad B \quad |B_j\rangle = |\dots,i_{N-1},i_N\rangle$$

Orthonormal basis: $\langle A_i | A_j \rangle = \langle B_i | B_j \rangle = \delta_{i,j},$ $\langle \alpha_i | \alpha_j \rangle = \langle \beta_i | \beta_j \rangle = \delta_{i,j}$

B

Schmidt coefficient: $\lambda_i \geq 0$

Relation between SVD and Schmidt decomposition

Singular value decomposition (SVD):

For a $K \times L$ matrix M,

$$M_{i,j} = \sum_{m} U_{i,m} \lambda_m V_{m,j}^{\dagger}$$

Singular values: $\lambda_m \geq 0$

 $\sum U_{i,m} U_{m,j}^{\dagger} = \delta_{i,j}$

Singular vectors:

$$\sum_{m}^{m} V_{i,m} V_{m,j}^{\dagger} = \delta_{i,j}$$

Relation to the Schmidt decomposition:

$$|\Psi\rangle = \sum_{i,j} M_{i,j} |A_i\rangle \otimes |B_j\rangle = \sum_{m} \lambda_m |\alpha_m\rangle \otimes |\beta_m\rangle$$

$$|\alpha_m\rangle = \sum_{i} U_{i,m} |A_i\rangle$$

$$|\beta_m\rangle = \sum_{i} V_{m,j}^{\dagger} |B_j\rangle$$

$$\langle \alpha_i |\alpha_j\rangle = \langle \beta_i |\beta_j\rangle = \delta_{i,j}$$

By using SVD, we can perform Schmidt decomposition.

Partial trace and reduced density matrix

For
$$\vec{x} \in \mathbb{V}_1 \otimes \mathbb{V}_2$$
 dim $\mathbb{V}_1 = n_1$, dim $\mathbb{V}_2 = n_2$ $|\vec{x}| = 1$

Density matrix:
$$\rho \equiv \vec{x}\vec{x}^{\dagger} \ (\rho_{ij} = x_i x_j^*)$$

(密度行列)
$$(\rho = |x\rangle\langle x|)$$
 *Note: rank $\rho = 1$

Orthonormal basis: $\{\vec{e}_1, \vec{e}_2, \dots, \vec{e}_{n_1}\} \in \mathbb{V}_1 \ \{\vec{f}_1, \vec{f}_2, \dots, \vec{f}_{n_2}\} \in \mathbb{V}_2$



Basis for \vec{x} : $\vec{g}_{i_1,i_2} = \vec{e}_{i_1} \otimes \vec{f}_{i_2}$

Index: $i = (i_1, i_2)$

Reduced Density matrix:

(縮約密度行列)

$$\rho_{\mathbb{V}_1} \equiv \mathrm{Tr}_{\mathbb{V}_2} \rho$$
 : a positive-semidefinite square matrix in \mathbb{V}_1

*Note: generally, rank $\rho_{\mathbb{V}_1} > 1$

$$(\rho_{\mathbb{V}_1})_{i_1,j_1} = \sum_{\underline{i_2}} \rho_{(i_1,\underline{i_2}),(j_1,\underline{i_2})}$$



Entanglement entropy

Entanglement entropy:

Reduced density matrix of a sub system (sub space):

Α

В

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi|$$









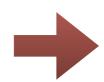




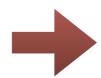
Entanglement entropy = von Neumann entropy of ρ_A

$$S = -\text{Tr}\left(\rho_A \log \rho_A\right)$$

Schmidt decomposition $|\Psi\rangle=\sum_{i}\lambda_{i}|\alpha_{i}\rangle\otimes|\beta_{i}\rangle$

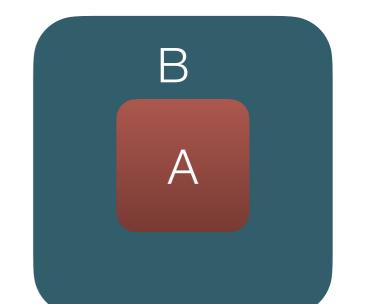


$$\rho_A = \sum_i \lambda_i^2 |\alpha_i\rangle \langle \alpha_i| \qquad \text{(*Exercise)}$$



$$S = -\sum_{i} \lambda_i^2 \log \lambda_i^2$$

$$(\sum_{i} \lambda_i^2 = 1)$$



Entanglement entropy is calculated through the spectrum of Schmidt coefficients.

(It also indicates $S = -\text{Tr}(\rho_B \log \rho_B)$)

Intuition for EE

Entanglement entropy is related to spectrum of singular values.

$$S=-{
m Tr}(
ho_A\log
ho_A)=-\sum_i\lambda_i^2\log\lambda_i^2$$
 = 1 Normalization: $(\sum\lambda_i^2=1)$

 $\operatorname{rank}\rho_A=1$

$$\lambda_1 = 1, \lambda_j = 0 \ (j \neq 1) \qquad \blacksquare \qquad S = 0$$



Flat spectrum

$$\lambda_1 = \lambda_2 = \dots = \lambda_n = \frac{1}{\sqrt{n}} \longrightarrow S = \log n$$

Exponential decay

$$\lambda_i \propto e^{-\alpha i}$$



$$S = 1 - \log 2\alpha \ (\alpha \ll 1, \alpha n \to \infty)$$

0.8

0 10 20 30

Smaller exponent gives larger entropy.

Intuition for EE: two S=1/2 spins

1.
$$|\Psi\rangle = |\uparrow\rangle \otimes |\downarrow\rangle$$



2.
$$|\Psi\rangle = \frac{1}{2}(|\uparrow\rangle - |\downarrow\rangle) \otimes (|\uparrow\rangle - |\downarrow\rangle)$$

Product state: S=0

Another product state $\lambda = 1$, S = 0

3.
$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle \right)$$



Spin singlet
$$\lambda_1 = \lambda_2 = \frac{1}{\sqrt{2}}$$
, $S = \log 2$

Maximally entangled State

4.
$$|\Psi\rangle = \left(x|\uparrow\rangle\otimes|\downarrow\rangle + \sqrt{1-x^2}|\downarrow\rangle\otimes|\uparrow\rangle\right)$$



Complicated state
$$\lambda_1 = |x|, \lambda_2 = \sqrt{1 - x^2}$$

 $S = x^2 \log x^2 + \sqrt{1 - x^2} \log(1 - x^2)$

Larger entanglement entropy ~ Larger correlation between two parts

Area law of the entanglement entropy in physics

General wave functions (vector):

EE is proportional to its **volume** (# **of qubits**).

$$S = -\text{Tr}\left(\rho_A \log \rho_A\right) \propto L^d$$

(c.f. random vector)

Ground state wave functions:

For a lot of ground states, EE is proportional to its area.



$$S = -\text{Tr} \left(\rho_A \log \rho_A \right) \propto L^{d-1}$$

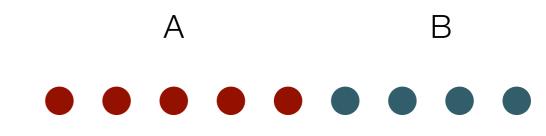
In the case of one-dimensional system:

Gapped ground state for local Hamiltonian

M.B. Hastings, J. Stat. Mech.: Theory Exp. P08024 (2007)

$$S = O(1)$$

Ground state are in a small part of the huge Hilbert space



Expected entanglement scaling for spin systems

Table 1Entanglement entropy scaling for various examples of states of matter, either disordered, ordered, or critical, with smooth boundaries (no corners).

Physical state	Entropy	Example
Gapped (brok. disc. sym.)	$aL^{d-1} + \ln(\deg)$	Gapped XXZ [143]
d = 1 CFT	$\frac{c}{3} \ln L$	$s = \frac{1}{2}$ Heisenberg chain [21]
$d \ge 2 \text{ QCP}$	$aL^{d-1} + \gamma_{\text{QCP}}$	Wilson–Fisher $O(N)$ [136]
Ordered (brok. cont. sym.)	$aL^{d-1} + \frac{n_{\rm G}}{2} \ln L$	Superfluid, Néel order [147]
Topological order	$aL^{d-1}-\gamma_{\mathrm{top}}$	\mathbb{Z}_2 spin liquid [159]

(Nicolas Laflorencie, Physics Reports 646, 1 (2016))

cf. free fermion

$$S \propto L^{d-1} \log L$$

For d ≥ 2, leading contribution satisfies area low even for gapless (critical) systems.

Exercise: examples of Schmidt decomposition

1-1: Random wave function (Sample code: Ex1-1.ipynb)

- Make a random vector
- SVD it and see singular value spectrum and EE

1-2: Ground state of the transverse field Ising model

$$\mathcal{H} = -\sum_{i=1}^{L-1} S_{i,z} S_{i+1,z} - \Gamma \sum_{i=1}^{L} S_{i,x}$$

(Sample code: Ex1-2.ipynb)

- Calculate GS by diagonalizing Hamiltonian
- SVD it and see singular value spectrum and EE

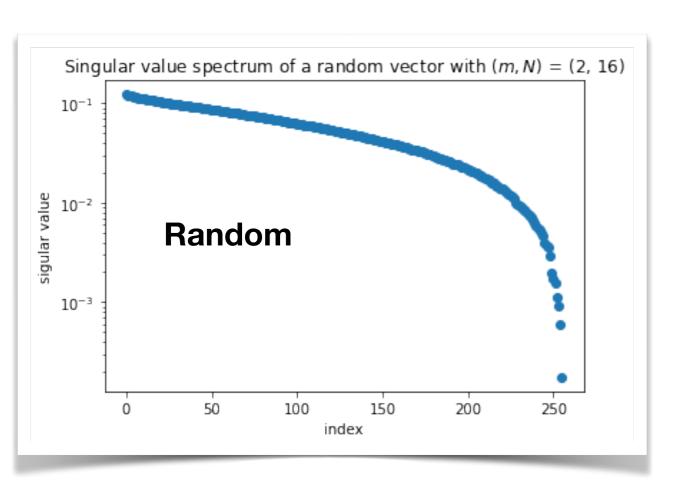
1-3: Picture image

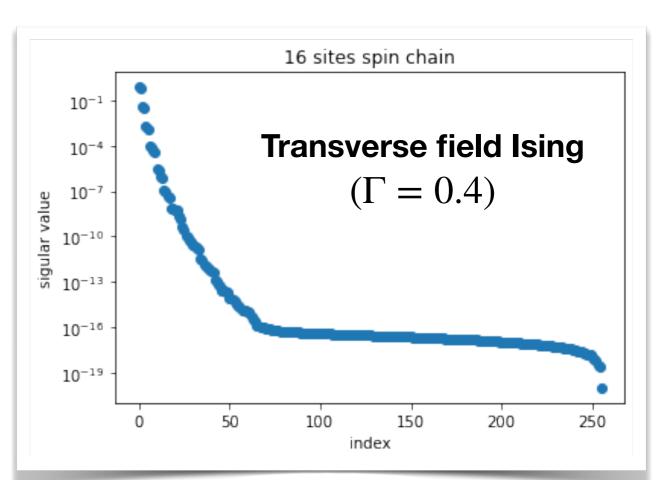
(Sample code: Ex1-3.ipynb)

- Transform an image data to the vector in m^N dimension.
- SVD it and see singular value spectrum and EE
 - * Try to simulate different system size "N"
 - * You can simulate other S by changing "m"

Spectrum for N=16 $\vec{v} \in \mathbb{C}^{2^{16}}$



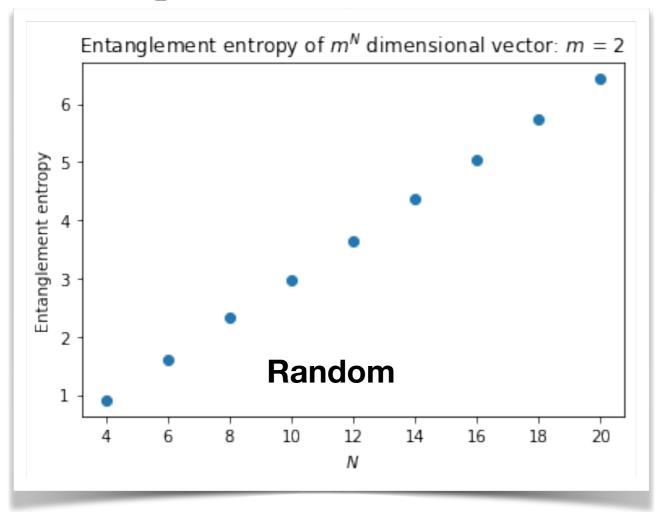


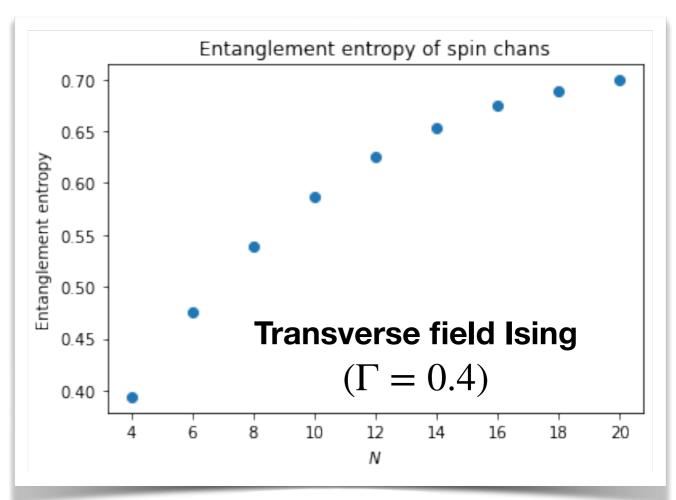


Ground state wave function has lower entanglement!

Scaling of the entanglement entropy

$$\vec{v} \in \mathbb{C}^{2^N}$$





Random vector: Volume low

Ground state: Area low

Exercises with Google Colab

I recommend you to use google colaboratory, https://colab.research.google.com where you can run .ipynb from your web browser.

When you use Google Colab, you need to also upload "ED.py"

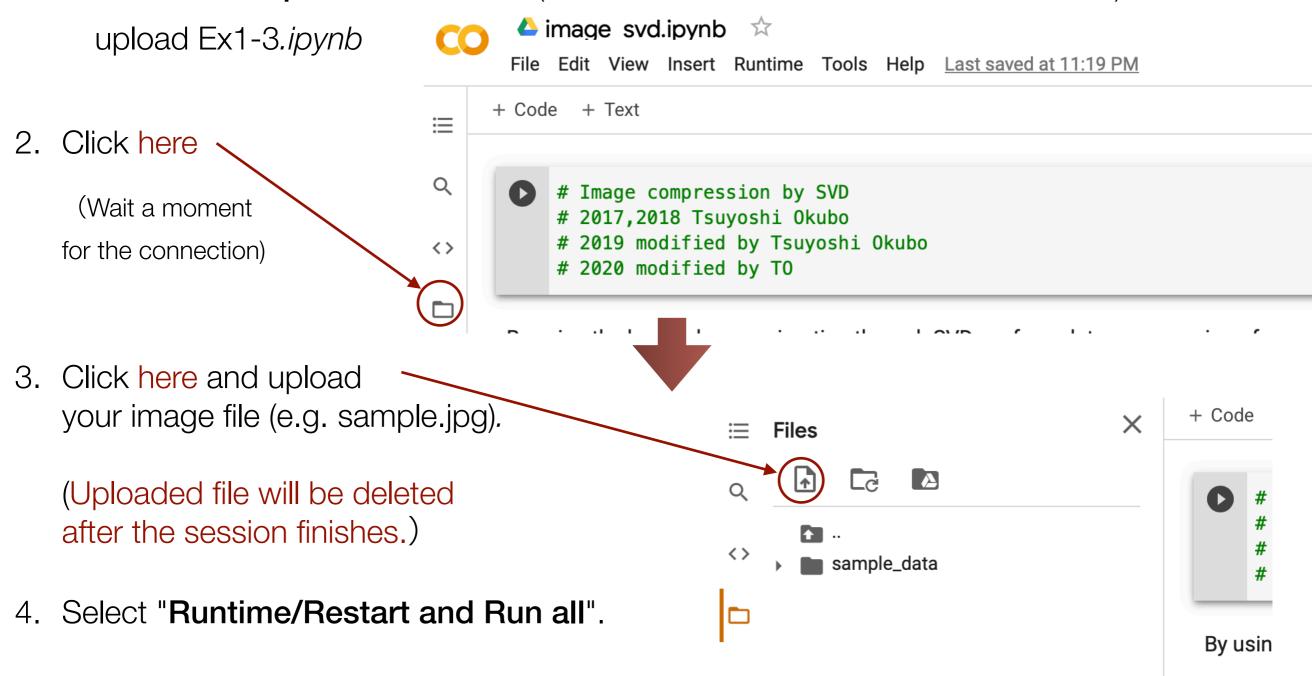
for the case of "Ex1-2.ipynb", and

your image file (sample.jpg),

for the case of "Ex1-3.ipynb".

How to use Google Colab

- 1. Open Ex1-3.ipynb in Google colab
 - ・ Select "**File/upload notebook**" ("ファイル/ノートブックをアップロード") and



Matrix product states (行列積状態)
(Tensor train decomposition)

Data compression of tensors (vectors)

Eg. General wave function:

$$|\Psi\rangle = \sum_{\{i_1, i_2, \dots i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

Coefficient vector can represent any points in the Hilbert space.



Ground states satisfy the area law.



In order to represent the ground state accurately, we might not need all of a^N elements.



Data compression by tensor decomposition:

Tensor network decomposition

*Same idea holds for any tensors.

Hilbert space



Tensor network decomposition (tensor network states)

Vector (or N-leg tensor):

$$\Psi_{i_1 i_2 \dots i_N}$$

 Ψ

of Elements = a^N

"Tensor network" decomposition



$$A_1[i_1]A_2[i_2]\cdots A_N[i_N] =$$

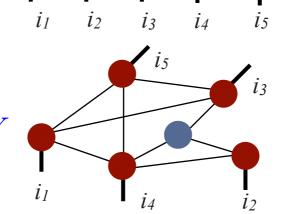
A[m]: Matrix for state m

* General network

$$\mathrm{Tr} X_{1}[i_{1}] X_{2}[i_{2}] X_{3}[i_{3}] X_{4}[i_{4}] X_{5}[i_{5}] Y$$

X,Y: Tensors

Tr: Tensor network contraction



By choosing a "good" network, we can express target vector efficiently.

ex. MPS: # of elements $=2ND^2$

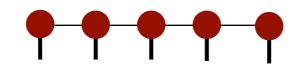
D: dimension of the matrix A

Exponential → Linear

*If D does not depend on N...

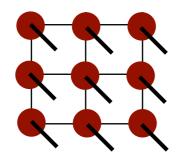
Examples of TNS

MPS:



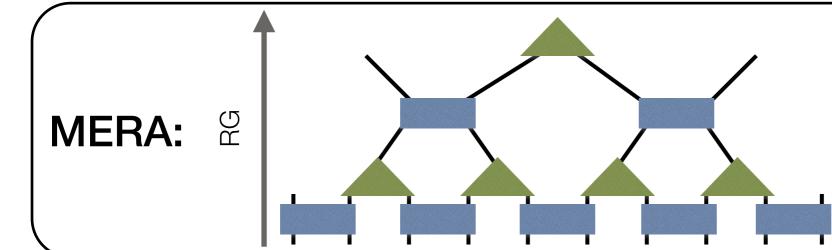
Good for 1d short range correlation (e.g. 1d gapped systems)

PEPS, TPS:



For higher dimensional correlation

Extension of MPS



Scale invariant systems

Good reviews:

Matrix product state (MPS)

(U. Schollwöck, Annals. of Physics **326**, 96 (2011))

(R. Orús, Annals. of Physics **349**, 117 (2014))

$$|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1i_2\ldots i_N} |i_1i_2\ldots i_N\rangle$$

$$\Psi_{i_1i_2\ldots i_N} \simeq A_1[i_1]A_2[i_2]\cdots A_N[i_N]$$

$$\simeq \Phi$$

$$A[i]: \text{Matrix for state } i$$

$$\frac{i}{m} = A_{ij}[m]$$

Note:

MPS is called "tensor train decomposition" in applied mathematics
 (I. V. Oseledets, SIAM J. Sci. Comput. 33, 2295 (2011))

A product state is represented by MPS with 1×1 "Matrix" (scalar)

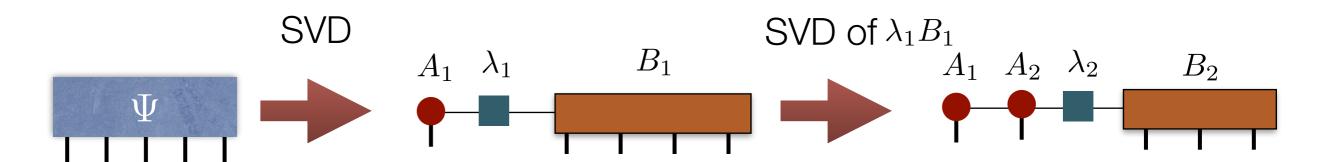
$$|\Psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots$$

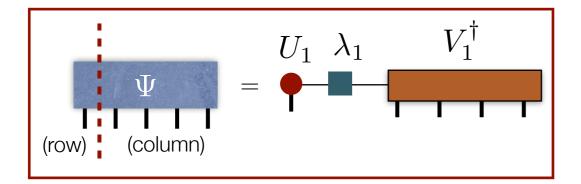
$$\Psi_{i_1 i_2 \dots i_N} = \phi_1[i_1]\phi_2[i_2] \cdots \phi_N[i_N]$$

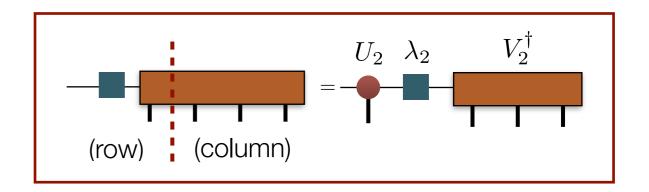
$$\phi_n[i] \equiv \langle i|\phi_i\rangle$$

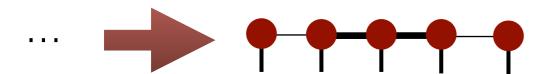
Matrix product state without approximation

General vectors can be represented by MPS exactly through successive Schmidt decompositions







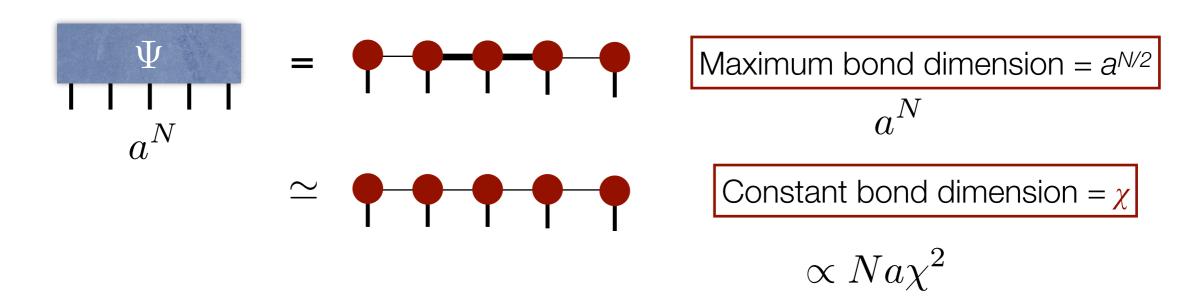


In this construction, the sizes of matrices depend on the position.

Maximum **bond dimension** = $a^{N/2}$

At this stage, no data compression.

Matrix product state: Low rank approximation

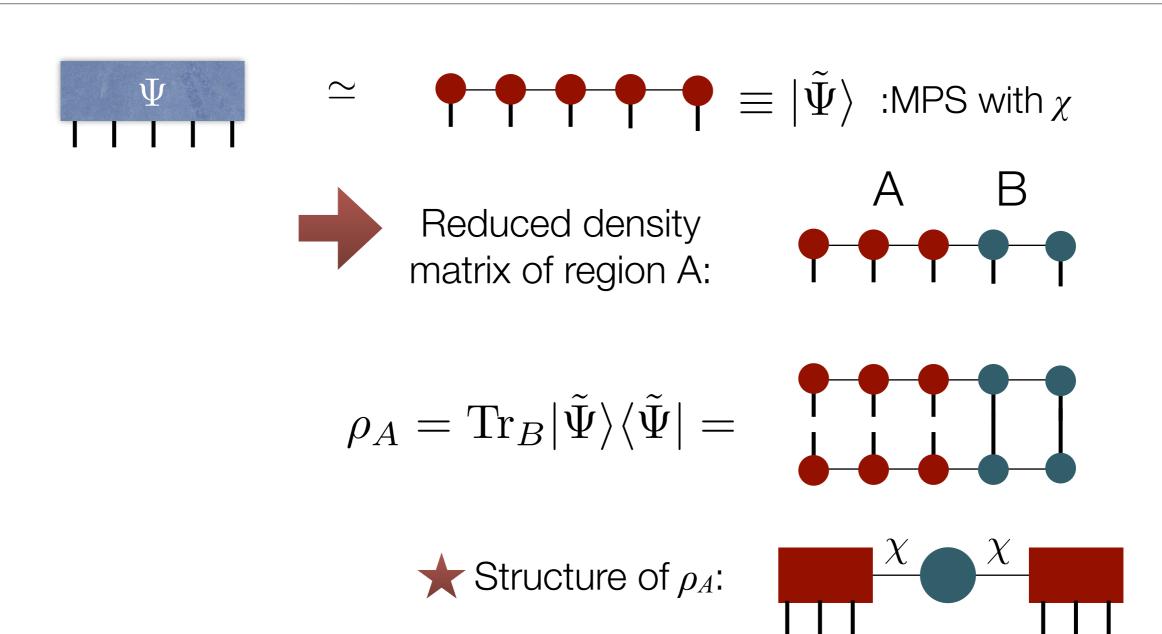


If the entanglement entropy of the system is O(1) (independent of N), matrix size " χ " can be small for accurate approximation.



On the other hand, if the EE increases as increase N, " χ " must be increased to keep the same accuracy.

Upper bound of Entanglement entropy







$$S_A = -\text{Tr } \rho_A \log \rho_A \leq \log \chi$$

Required bond dimension in MPS representation

$$S_A = -\text{Tr } \rho_A \log \rho_A \le \log \chi$$



The upper bound is independent of the "length".

length of MPS \Leftrightarrow size of the problem n



EE of the original vector	Required bond dimension in MPS representation
$S_A = O(1)$	$\chi = O(1)$
$S_A = O(\log N)$	$\chi = O(N^{\alpha})$
$S_A = O(N^{\alpha})$	$\chi = O(c^{N^{\alpha}})$

$$(\alpha \leq 1)$$

Next week

1st: Huge data in modern physics (Today)

2nd: Information compression in modern physics

(+review of linear algebra)

3rd: Review of linear algebra (+ singular value decomposition)

4th: Singular value decomposition and low rank approximation

5th: Basics of sparse modeling

6th: Basics of Krylov subspace methods

7th: Information compression in materials science

8th: Accelerating data analysis: Application of sparse modeling

9th: Data compression: Application of Krylov subspace method

10th: Entanglement of information and matrix product states

11th: Matrix product states + Application of MPS to eigenvalue problems

12th: Application of MPS to time evolution and data science

13th: Other tensor network representations

+ (Appendix: Information compression by tensor network renormalization)