A numerical introduction to tensor networks for quantum simulation

Austin Minnich, California Institute of Technology
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[Credit for course materials: Prof. Jan von Delft]

1. Why tensor networks?

Tensor networks provide a flexible description of quantum states.

In some cases, they are efficient - can accurately describe state with polynomial resources.

Example: spin- chain, with sites:

Local state space of site :

Local state label:

Local dimension:

Shorthand:

Index on state label suffices to identify the site Hilbert space

Generic basis state for full chain of length N
(convention: add state spaces for new sites from left):

Hilbert space for full chain:

Generic quantum state:

Dimension of full Hilbert space : (# of different configurations of)

Specifying involves specifying , i.e. different complex numbers.

is a tensor of rank (rank = # of legs)

Graphical representation: (one leg for each index)

Claim: such a rank L tensor can be represented in many different ways:

MPS: matrix product state

PEPS: projected entangled-pair state

arbitrary tensor network

-a link between two sites represents entanglement between them

-different representations -> different entanglement book-keeping

-tensor network = entanglement representation of a quantum state

2. Iterative diagonalization

Consider a spin-s chain with Hamiltonian

local state space for site :

We seek eigenstates of :

Diagonalize Hamiltonian iteratively, adding one site at a time.

N = 1: Start with first site, diagonalize in Hilbert space . Eigenstates have form

(sum over implied) coefficient matrix combining ‘incoming’ into ‘outgoing’

N = 2: Add second site, diagonalize in Hilbert space :

(sum over implied) coefficient matrix combining ‘incoming’ into ‘outgoing’

N = 3: Add third site, diagonalize in Hilbert space :

Your try:

Answer:

Continue similarly until having added site N. Eigenstates of have following structure:

Nomenclature: = physical indices, = (virtual) bond indices

Alternative, widely-used notation: ‘reshape’ coefficient tensors as

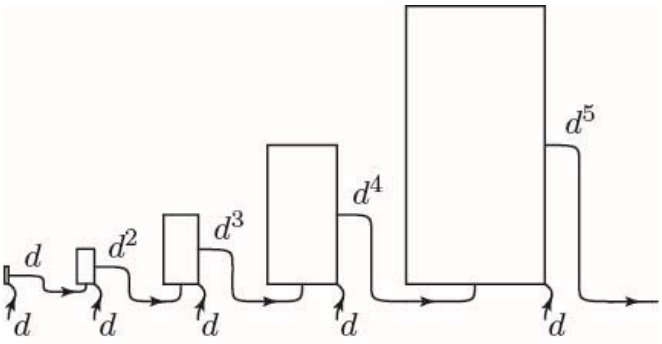
to highlight ‘matrix product’ structure in noncovariant notation:

Comments

1. Iterative diagonalization of 1D chain generates eigenstates whose wave functions are tensors that are expressed as matrix products -> matrix product states (MPS)

Matrix size grows exponentially.

for given	,	has dimension	(vector)
for given	,	has dimension	(rectangular matrix)
for given	,	has dimension	(larger rectangular matrix)

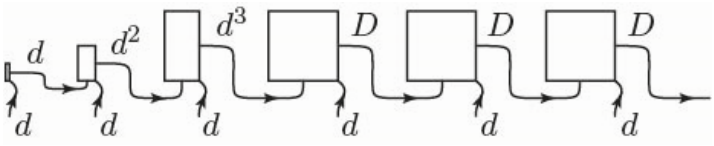


“Hilbert space is a large place!”

Numerical costs explode with increasing N, so truncation schemes are needed.

Truncation can be done in a controlled way using tensor network methods.

Standard truncation scheme: use for all virtual bonds



2. Number of parameters available to encode state:

[equal if all virtual bonds have same dimension D]

If N is large:

Why should we expect this ansatz with polynomial parameters to accurately represent a quantum state?

Remarkable fact: for 1d Hamiltonian with local interactions and a gapped spectrum, its ground state can be accurately represented by MPS!

Reason: Area law for entanglement entropy. We will discuss later.

3. Covariant index notation

More detail of covariant index notation is in L2 & L10 of “Mathematics for Physicists”, Altland & von Delft, see here.

Kets (Hilbert space vectors)

For kets, indices are down. E.g. basis kets:

For components of kets (wrt a basis), indices are upper:

Repeated indices (always up-down pairs) are always summed (implied summation).

Example: linear combination of kets.

Note: for the index identifies components of kets -> upper

the index identifies components of basis kets -> lower

Basis for direct product space:

Note ket order: start with first space on very right, successively attach new spaces from left.
Linear combinations:

Bras (Hilbert space dual vectors)

For bras, indices are upper. E.g. basis bras:

For components of bras (wrt a basis), indices are lower:

Complex conjugation:

Linear combinations of bras:

Complex conjugation:

Note: for , the index identifies basis bras (dual vectors) hence upper

the index identifies components of bras (dual vectors) hence lower

Basis for direct product space:

Note bra order: opposite to kets so expectation values yield nested bra-ket pairs:

Linear combinations:

Complex conjugation:

Orthonormality

If form orthonormal basis:

If form orthonormal basis, too:

Combined:

Hence A is unitary:

Operators

Simplified notation

It is customary to simplify notational conventions for kets and bras.

In kets, use subscript indices as ket names:

In bras, use superscript indices as bra names:

Now up/down convention for indices is no longer displayed but it still implicit!

Linear combination of kets:

Coefficient matrix = overlap:

If direct products are involved:

Coefficient matrix = overlap:

Linear combination of bras:

Coefficient matrix = overlap:

If direct products are involved:

Coefficient matrix = overlap:

Operators:

In the overlaps:

bra indices: upper on or , as incoming arrows

ket indices: lower on or , as outgoing arrows

4. Entanglement entropy and Area Laws (introductory comments)

Consider a quantum system in state , with density matrix

Divide system into two parts, . Suppose has linear dimension .

To obtain reduced density matrix of (or), trace out (or)

'reduced density matrix' for :

'Entanglement entropy' of and :

Key result: for Hamiltonians with only local interactions, ground state is governed by an 'area law':

(area of boundary of)

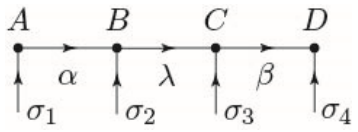
in 3D for gapped system

in 2D for gapped system

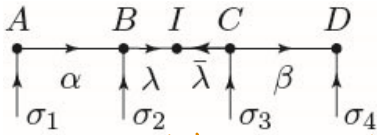
in 1D for gapped system

in 1D for *gapless system

Now consider an MPS of maximal bond dimension D:



Divide system into two parts: Left -> 2 sites, Right -> 2 sites



=entangled superposition of two state spaces,
each having dimension of at most D

(After the sum over has been performed explicitly using
Kronecker delta, result contains non-covariantly paired indices

Density matrix:

Reduced density matrix:

with matrix elements

This matrix has rank (say)

Let be its eigenvalues, with

and normalization

Entanglement entropy:

Maximal if for all :

1D gapped:

1D critical:

2D gapped:

3D gapped:

Conclusion: MPS can encode ground state efficiently for gapped and gapless systems in 1D, but not 2D or 3D!

5. Tensor network diagrams

[Orus 2014, Sec 4.1]

'tensor' = multi-dimensional array of numbers

'rank of tensor' = number of indices = # of legs

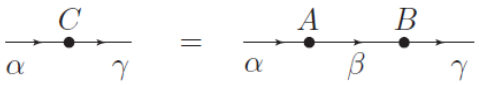
rank-0: scalar

rank-1: vector

rank-2: matrix

rank-3: tensor

Index contraction: summation over repeated index



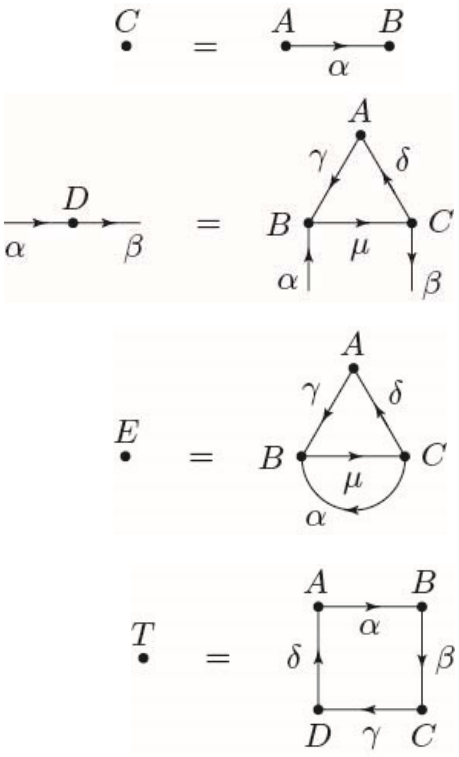
graphical representation of matrix product

= ‘bond dimension’ of index

‘open index’ = non-contracted index (here)

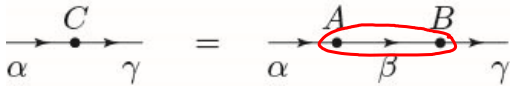
‘tensor network’ = set of tensors with some or all indices contracted according to some pattern

Examples:



Cost of computing contractions

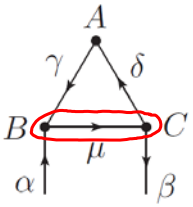
Result of contraction does not depend on order in which indices are summed, but numerical cost does!

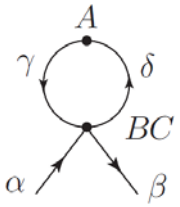
Example 1: cost of matrix multiplication is 

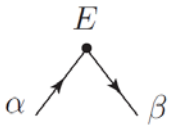
For every fixed and (combinations), sum over values of

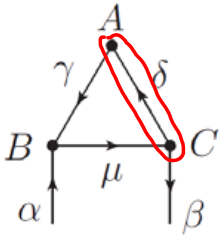
Cost = (simplifies to if all bond dimensions are)

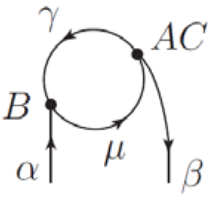
Example 2:

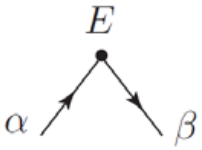












First contraction scheme has total cost , second has !

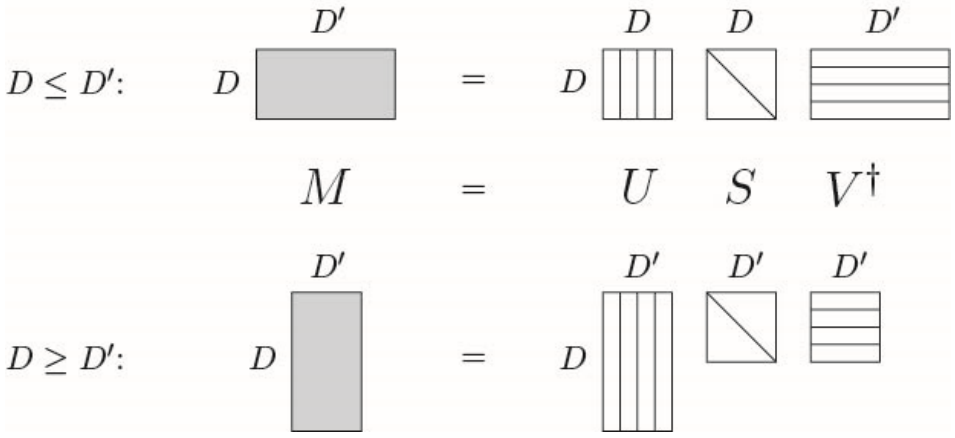
Finding optimal contraction order is difficult. In practice, trial and error….

In first part of course we will focus on 1D tensor networks, then 2D.

6. Singular value decomposition (SVD)

[Schollwoeck2011, Sec 4]

Any matrix of dimension can be written as



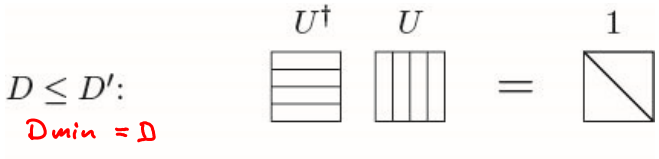
Properties of S

- square matrix of dimension
- diagonal with non-negative diagonal elements (singular values)
- Schmidt rank : number of non-zero singular values

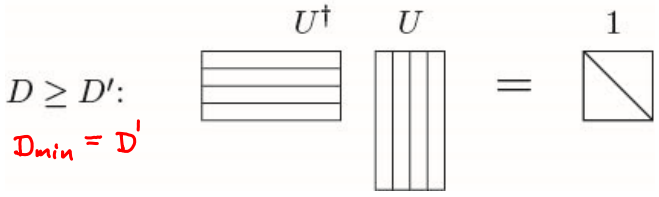
- arrange in descending order:

Properties of :

- matrix of dimension



$D_{min} = D$

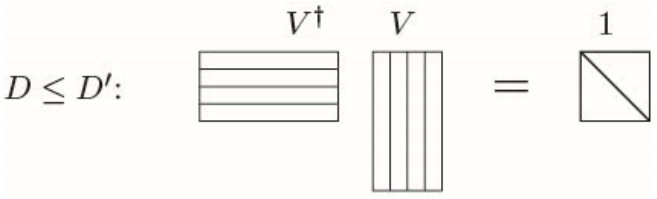


$D_{min} = D'$

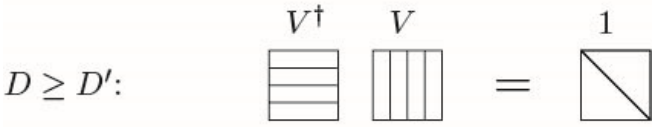
- columns are orthonormal

Properties of :

- matrix of dimension



- rows are orthonormal



Useful properties:

So columns of are eigenvectors of

Columns of are eigenvectors of

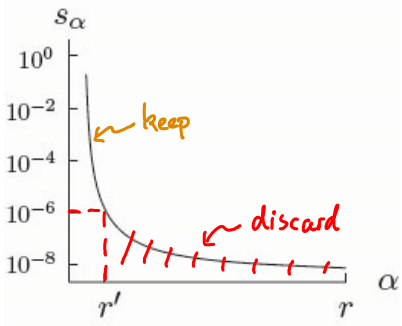
Truncation

SVD yields optimal approximation of rank matrix by a rank matrix

(optimal wrt Frobenius norm)

Suppose

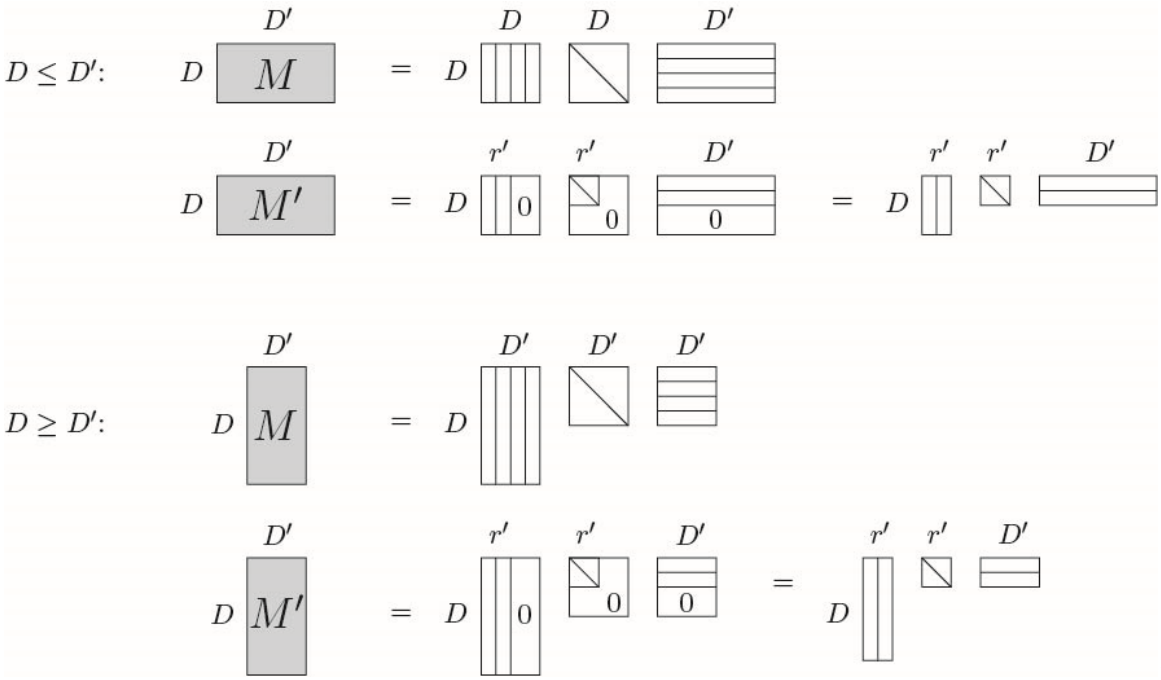
with



Truncate:

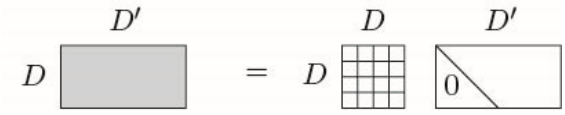
with

Retain only largest singular values! Visualization, with :

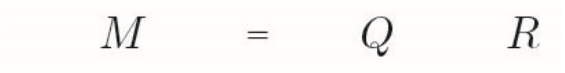


QR decomposition

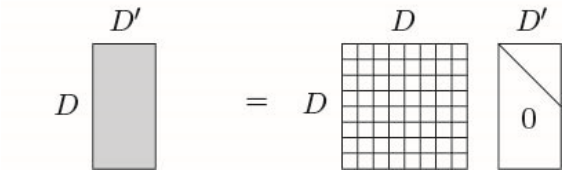
If singular values are not needed,



a matrix



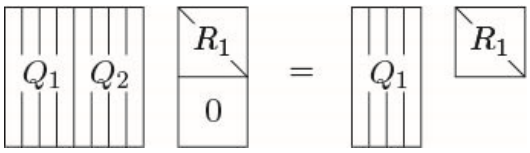
has the ‘full QR decomposition’



with a unitary matrix

and a upper triangular matrix

If $D \geq D'$, then M has the ‘thin QR decomposition’



with dim(Q1) = , dim(R1) = ,

and R1 upper triangular.

QR is numerically cheaper than SVD but has less information (does not provide rank).