25tn:Tensor Networks for Many-Body Physics and Beyond:

Jan von Delft

TNB.0

Why study tensor networks? Because tensor networks provide a powerful way of compressing information: Tensors with many legs represent vectors in high-dimensional spaces. If they are compressible, they can be expressed through networks of tensors with only a few (2, 3, 4) legs. This representation greatly reduced the numerical cost of computations performed with such tensors.

In quantum mechanics, wave-functions of many-body systems are high-dimensional tensors. Tensor networks offer a powerful language for encoding the wave functions of quantum many-body states, and the operators acting on them, in terms of contractions of tensors. They encode entanglement between subsystems in the bonds linking the tensors of the network.

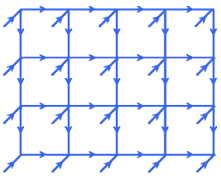
Recent progress has utilized the notion of the tangent space to a given tensor network state: the vector space of one-site variations of the given state. Tangent space methods provide a convenient framework for describing small changes of a given reference state (e.g. during energy minimization or time evolution).

More generally, any function of many variables can, via discretization of the variables, be represented as a high-dimensional tensor. If this tensor is compressible, the function can be expressed through a tensor network. Then standard operations on functions, such as addition, multiplication, integration, convoulation, Fourier transformation, can all be performed using tensor network methodology, often at greatly reduced numerical costs.

This course will provide an introduction to tensor networks and tangent space methods, and how they are used to compute ground states, time evolution, dynamical spectral functions, and more generally, to compress and manipulate multivariate functions.

Course outline:

1. Tensor network basics (TNB)
2. Matrix product states (MPS)
3. Density matrix renormalization group (DMRG)
4. Tangent space (TS)
5. Time evolution: time-dependent variational principle (TDVP)
6. Controlled Bond expansion (CBE)
7. Dynamical correlators (DC)
8. Tensor cross interpolation (TCI)
9. Two-dimensional tensor networks (PEPS)



Course website is on Moodle:
https://moodle.lmu.de/course/view.php?id=40399

References: consult the bibtex file TensorNetworkLiterature.bib on course website → References

These lecture notes are based on a course on 'Tensor Networks' taught at Ludwig Maximilian University, summer semester 2023: for lecture notes, tutorial exercises and videos for that '23tn', see:
https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_23/tensor_networks_23/index.html

In the present course, I will occasionally reference parts of the tn23 course, e.g.
tn23:L01.3 refers to lecture L01, part 3. Its video, numbered 01.3, can be found here:

https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_23/tensor_networks_23/videos/index.html

First few lectures:Tensor networks basics (TNB)

1. Why matrix product states (MPS)?
2. Covariant index notation
3. Tensor network diagrams
4. Unitaries and isometries
5. Singular value decomposition
6. Schmidt decomposition

1. Why matrix product states?

TNB.1

Consider a generic quantum chain model

with L sites, enumerated by an index $\ell = 1, \ldots, L$

Local Hilbert space of site ℓ : $V = \{|\sigma_\ell\rangle\}$, $\dim(\sigma_\ell) = d$ ← local dimension (1)

Examples: spin s: $V = \{|-s\rangle, |-s+1\rangle, \ldots, |s-1\rangle, |s\rangle\}$, $d = 2s+1$ (2a)

spinful fermions: $V = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$, $d = 4$ (2b)

Local product basis for full system of L sites (convention: add state spaces for new sites from the right):

$$|\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \ldots \otimes |\sigma_\ell\rangle \otimes \ldots |\sigma_L\rangle := |\sigma_1, \sigma_2, \ldots, \sigma_\ell, \ldots, \sigma_L\rangle := |\vec{\sigma}\rangle_L \quad (3)$$

← identifies length of chain

Hilbert space for full chain: $\mathcal{H}^L = \mathrm{span}\{|\vec{\sigma}\rangle_L\} = V^{\otimes L} = V$ (4)

Dimension of full Hilbert space $\mathcal{H}^L$: d^L (# of different configurations of $\vec{\sigma}_L$) (5)

General quantum state: $|\psi\rangle = \sum_{\sigma_1 \ldots \sigma_L} |\sigma_1, \ldots, \sigma_L\rangle \psi^{\sigma_1, \ldots, \sigma_L} := |\vec{\sigma}\rangle \psi^{\vec{\sigma}}$ (6)

$(\in V)$

wavefunction

arbitrary linear combinations

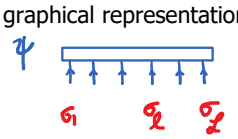
summation over repeated indices implied

Specifying $|\psi\rangle$ involves specifying $\psi^{\vec{\sigma}} \in \mathbb{C}^{d^L}$, i.e. d^L different complex numbers.

$\psi^{\vec{\sigma}} = \psi^{\sigma_1, \ldots, \sigma_L}$ is a tensor of degree L (7)

← number of legs

graphical representation

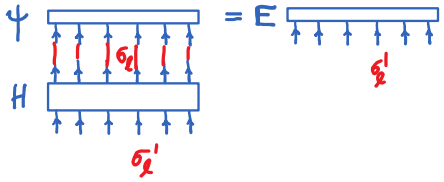


Schrödinger equation: operator . ket = ket $\hat{H}|\psi\rangle = E|\psi\rangle$ (8)

In local basis: $\langle\vec{\sigma}'|(8)$ $\langle\vec{\sigma}'|\hat{H}|\vec{\sigma}\rangle\langle\vec{\sigma}|\psi\rangle = E\langle\vec{\sigma}'|\psi\rangle$ (9)

implicit Einstein summation $\sum_{\vec{\sigma}}$ over repeated 'local indices' (indicated diagrammatically by connecting legs)

Schrödinger equation: $[H]^{\vec{\sigma}'}_{\vec{\sigma}} \psi^{\vec{\sigma}} = E \psi^{\vec{\sigma}'}$ (10)



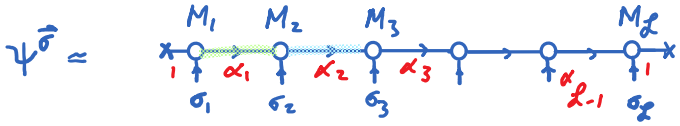
matrix . vector = vector $\left(d^L \times d^L\right)\left(d^L\right) = E\left(d^L\right)$ (11)

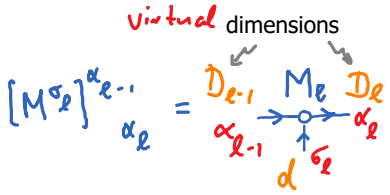
When H and ψ are viewed as matrices and vectors, they have exponentially many components.

Direct diagonalization not possible for $L \gtrsim 30$ 'Curse of dimensionality' !

Fact (F1): any $\psi^{\vec{\sigma}}$ =  can expressed as a 'matrix product state' (see MPS.1):

'factorized' or 'unfolded'

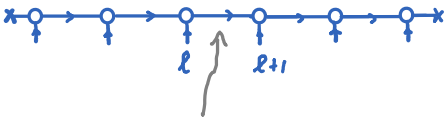




$$= [M_1^{\sigma_1}]^{1}_{\alpha_1} [M_2^{\sigma_2}]^{\alpha_1}_{\alpha_2} [M_3^{\sigma_3}]^{\alpha_2}_{\alpha_3} \cdots [M_\ell^{\sigma_\ell}]^{\alpha_{\ell-1}}_{1} = \prod_{\ell=1}^{\mathcal{L}} M_\ell^{\sigma_\ell} \qquad (12) \qquad D_0 = D_\mathcal{L} = 1$$

implicit Einstein summation $\sum_{\alpha_1 \alpha_2 \ldots \alpha_{\ell-1}}$ over repeated 'virtual bond' indices $\alpha_\ell = 1, \ldots, D_\ell$ (indicated diagrammatically by connecting legs)

MPS representation reveals entanglement properties of $\psi^{\vec{\sigma}}$: Link between neighboring sites encodes the entanglement between them (see TNB.6)



Fact (F2): Entanglement entropy between sites ℓ and $\ell+1$ [see (TNB6.16)]: $S_\ell \leq \log_2 D_\ell$ (13)

$\Rightarrow$ bond dimension needed to encode S_ℓ grows exponentially with S_ℓ: $D_\ell \gtrsim 2^{S_\ell}$ (14)

Memory footprint of MPS is $\mathcal{O}(\mathcal{L} d D^2)$ where $D = \max\{D_\ell\}$ = 'rank' of $\psi^{\vec{\sigma}}$ (15)

A generic $\psi^{\vec{\sigma}}$ has an exponentially large rank, $D \sim d^{\mathcal{L}/2}$ (16)

But there are exceptions: $\psi^{\vec{\sigma}}$ is called compressible if its rank does not grow exponentially with $\mathcal{L}$.

Fact (F3): for 1-dimensional systems, ground state wave functions of local Hamiltonians with short-ranged interactions are compressible. Therefore, they can be encoded using MPS with only polynomial costs in system size: $\mathcal{O}(\mathcal{L} d D^2)$

$\mathbb{C}^{d^\mathcal{L}}$ huge space of all tensors of degree $\mathcal{L}$

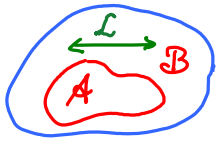
tiny space of compressible tensors

Intermezzo: (F3) follows from 'area law'.

Consider quantum system in pure state $|\psi\rangle$, with density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$

Divide system into two parts, $\mathcal{A}$ and $\mathcal{B}$. Suppose $\mathcal{A}$ has linear dimension $\mathcal{L}$. (number of sites)

To obtain reduced density matrix of $\mathcal{A}$ (or $\mathcal{B}$), trace out $\mathcal{B}$ (or $\mathcal{A}$):



'reduced density matrix' for $\mathcal{A}$: $\hat{\rho}_\mathcal{A} := \mathrm{Tr}_\mathcal{B} \hat{\rho}$ and $\hat{\rho}_\mathcal{B} := \mathrm{Tr}_\mathcal{A} \hat{\rho}$ (17)

'Entanglement entropy' of $\mathcal{A}$ and $\mathcal{B}$: $S_{\mathcal{A}/\mathcal{B}} = -\mathrm{Tr}\, \hat{\rho}_\mathcal{A} \log_2 \hat{\rho}_\mathcal{A} = -\sum_\alpha w_\alpha \log_2 w_\alpha$ (18) (eigenvalues of $\hat{\rho}_\mathcal{A}$)

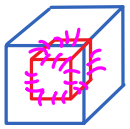
Fact (F4): For Hamiltonians with only local interactions, the ground state entanglement entropy between subsystems $\mathcal{A}$ and $\mathcal{B}$ is governed by an 'area law' Hastings2007,Eisert2010,Cirac2021]:

bond dimension needed for (14):

between subsystems A and B is governed by an 'area law' Hastings2007,Eisert2010,Cirac2021]:

bond dimension needed for (14):

$S_{A/B} \sim$ (area of boundary of A)

$\sim L^2$ in 3D for gapped system  $\Rightarrow \sim 2^{L^2}$

$\sim L$ in 2D for gapped system  $\Rightarrow \sim 2^{L}$

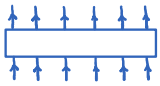
$\sim$ const. $+ \ln L$ in 1D for gapless system  $\Rightarrow \sim L$

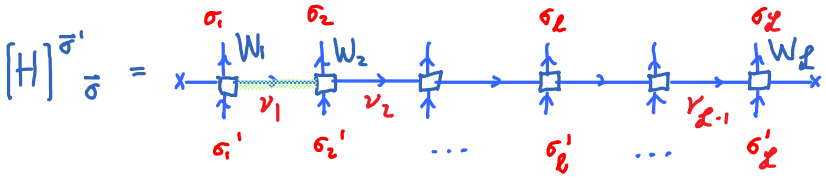
$\sim$ const. in 1D for gapped system  $\Rightarrow \sim$ const.

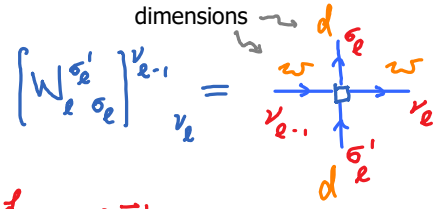
$D \gtrsim 2^{S_{A/B}}$ (14)

For 1D cases, bond dimension does not grow exponentially with system size

$\Rightarrow$ ground state wave functions are compressible!

Fact (F5): any Hamiltonian $[H]^{\vec{\sigma}'}_{\vec{\sigma}}$ =  can be expressed as a matrix product operator (MPO):



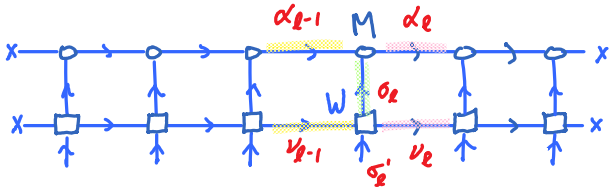
dimensions 

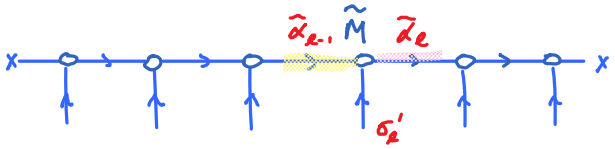
$$= [W_1^{\sigma_1'\sigma_1}]^{1}_{\nu_1} [W^{\sigma_2'\sigma_2}]^{\nu_1}_{\nu_2} \cdots [W^{\sigma_L'\sigma_L}]^{\nu_{L-1}}_{1} = \left[\prod_{\ell=1}^{L} W_\ell\right]^{\vec{\sigma}'}_{\vec{\sigma}} \quad (20)$$

implicit Einstein summation $\sum_{\nu_1,\nu_2 \cdots \nu_{L-1}}$ over repeated 'MPO bond' indices $\alpha_\ell = 1, \ldots, w$ (indicated diagrammatically by connecting legs)

Fact (F5): for generic short-ranged Hamiltonian, MPO bond dimension is $\dim(w) = O(1)$
thus, such Hamiltonians are 'compressible'. e.g. 3 or 5

Application of MPO to MPS yields another MPS: $\tilde{\psi}^{\vec{\sigma}'} = [H]^{\vec{\sigma}'}_{\vec{\sigma}} \psi^{\vec{\sigma}}$ (21)



$=$ 

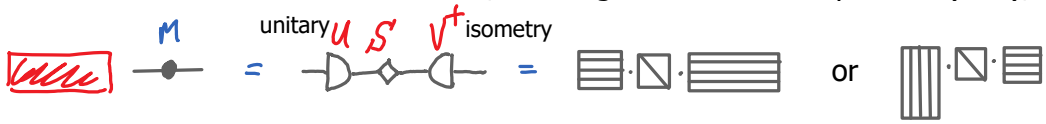
$$[\tilde{M}_\ell^{\sigma_\ell'}]^{\tilde{\alpha}_{\ell-1}}_{\tilde{\alpha}_\ell} = [W_\ell^{\sigma_\ell'\sigma_\ell}]^{\nu_{\ell-1}}_{\nu_\ell} [M_\ell^{\sigma_\ell}]^{\alpha_{\ell-1}}_{\alpha_\ell}$$

with composite indices, $\tilde{\alpha}_{\ell-1} = (\alpha_{\ell-1}, \nu_{\ell-1})$, $\tilde{\alpha}_\ell = (\nu_\ell, \nu_\ell)$ (22)

of increased dimension: $\tilde{D}_\ell = D_\ell \cdot w$ (23)

Computational cost of evaluating MPO . MPS is $O(L d^2 D^2 w^2)$

i.e. not exponential but polynomial in system size! This is why we love working with MPOs and MPSs.
However, since bond dimensions grow with every MPO application, we need to truncate bonds.
To do this with minimal information loss, use singular value decomposition (SVD), see TNB.4.



2. Arrow conventions

TNB.2

Premise: in Linear Algebra, vectors and dual vectors are notationally distinguished by lower/upper placement of indices ('covariant notation'). E.g. to describe linear transformation applied to basis vectors:

basis vectors: $\{|e_\sigma\rangle\}$ transformed vectors: $\{|v_\alpha\rangle = |e_\sigma\rangle T^\sigma{}_\alpha\}$ (1)

dual basis vectors: $\{\langle e^\sigma|\}$ transformed dual vectors: $\{\langle v^\alpha| = T^\dagger{}^\alpha{}_\sigma \langle e^\sigma| = \overline{T^\sigma{}_\alpha}\}$ (2)

Indices of coefficients are placed such that summed indices come in high-low pairs.

See, chap. L2 & L10 of "Mathematics for Physicists", Altland & von Delft, www.cambridge.org/altland-vondelft

In Quantum Mechanics, kets are vectors, bras are dual vectors, but low/high index placements are not customary. However, I do find it useful to do so when working with tensor networks, where very many indices arise, and high/low placements help to remember which indices can be contracted.
In diagrams for coefficient tensors, high/low indices on coefficient tensors are distinguished by in/out arrows.

Shorthand notation for kets: $|\sigma\rangle = |e_\sigma\rangle$ (basis vectors), $|\alpha\rangle = |v_\alpha\rangle$ (transformed vectors)

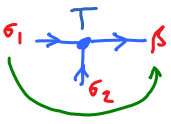
Shorthand notation for bras: $\langle\sigma| = \langle e^\sigma|$ (dual basis vectors), $\langle\alpha| = \langle v^\alpha|$ (transformed dual vectors)

Linear combination of kets: $|\alpha\rangle = |\sigma\rangle T^\sigma{}_\alpha$ shorthand for $= |e_\alpha\rangle T^\sigma{}_\alpha$

(3)

Coefficient matrix = overlap: $T^\sigma{}_\alpha = \langle\sigma|\alpha\rangle$ (4)

If direct products are involved: $|\beta\rangle = |\sigma_1\rangle\otimes|\sigma_2\rangle T^{\sigma_1\sigma_2}{}_\beta$
add new spaces on the right

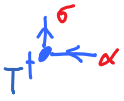


(5)

Coefficient matrix = overlap: $T^{\sigma_1\sigma_2}{}_\beta = \langle\sigma_2|\otimes\langle\sigma_1|\beta\rangle$
note bra order: opposite to that of kets in (5)

index-reading order (6)

Linear combination of bras: $\langle\alpha| = T^\dagger{}^\alpha{}_\sigma\langle\sigma| = \overline{T^\sigma{}_\alpha}\langle e^\sigma|$ shorthand for

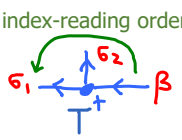


(7)

Coefficient matrix = overlap: $T^\dagger{}^\alpha{}_\sigma = \langle\alpha|\sigma\rangle = \overline{\langle\sigma|\alpha\rangle} \overset{(4)}{=} \overline{T^\sigma{}_\alpha}$ (8)

index-reading order

If direct products are involved: $\langle\beta| = T^\dagger{}^\beta{}_{\sigma_2\sigma_1}\langle\sigma_2|\otimes\langle\sigma_1|$



(9)

Coefficient matrix = overlap: $T^\dagger{}^\beta{}_{\sigma_2\sigma_1} = \langle\beta|\sigma_1\rangle\otimes|\sigma_2\rangle = \overline{\langle\sigma_2|\otimes\langle\sigma_1|\beta\rangle} \overset{(6)}{=} \overline{T^{\sigma_1\sigma_2}{}_\beta}$ (10)

Operators: $\hat{O} = |\vec{\sigma}'\rangle O^{\vec{\sigma}'}{}_{\vec{\sigma}}\langle\vec{\sigma}|$, $O^{\vec{\sigma}'}{}_{\vec{\sigma}} = \langle\vec{\sigma}'|\hat{O}|\vec{\sigma}\rangle = \langle e^{\vec{\sigma}'}|\hat{O}|e_{\vec{\sigma}}\rangle$

(11)

In all these overlaps (3,5,7,9):

bra indices: sitting high on T or $T^\dagger$, depicted by incoming arrows
ket indices: sitting low on T or $T^\dagger$, depicted by outgoing arrows

3. Tensor network diagrams

[Orus 2014, Sec. 4.1]

TNB.3

'tensor' = multi-dimensional array of numbers

'~~rank of~~ degree' = number of indices = # of legs

'dimension of leg' = number of values taken by its index, $\alpha = 1, \dots, D_\alpha$

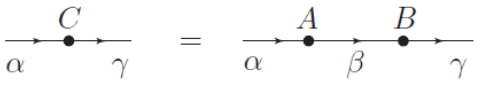
overbar denotes complex conjugation

degree-0:	scalar	A		$A^\dagger := \bar{A}$
degree-1:	vector	A^σ		$A^\dagger{}_\sigma := \overline{A^\sigma}$
degree-2:	matrix	$A^\sigma{}_\alpha$		$A^{\dagger\alpha}{}_\sigma := \overline{A^\sigma{}_\alpha}$
degree-3:	tensor	$A^{\alpha\sigma}{}_\beta$		$A^{\dagger\beta}{}_{\sigma\alpha} := \overline{A^{\alpha\sigma}{}_\beta}$

[Reminder: Conventions for using arrows and distinguishing between super- and subscripts ('covariant notation') are explained in TNB.2. In short: on coefficient tensors, incoming = high, outgoing = low. Use of covariant notation is not customary in tensor network literature - most authors write all indices low.]

Index contraction: summation over repeated index

$$C^\alpha{}_\gamma = \sum_{\beta=1}^{D_\beta} A^\alpha{}_\beta B^\beta{}_\gamma \equiv A^\alpha{}_\beta B^\beta{}_\gamma$$



graphical representation of matrix product

D_β = 'bond dimension' of index β

(depends on context, can be different for each index; the subscript β on D_β is often/usually not written explicitly)

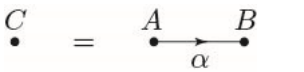
'open index' = non-contracted index (here α , γ)

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

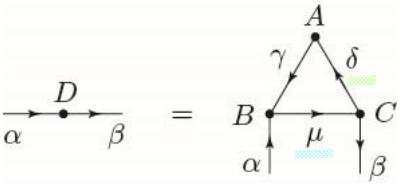
Examples:

$C = A_\alpha B^\alpha$

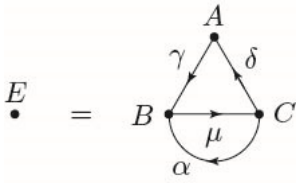
scalar dual vector · vector



$D^\alpha{}_\beta = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^\mu{}_{\beta\delta}$

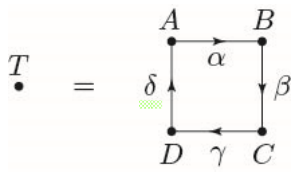


$E = D^\alpha{}_\alpha = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^\mu{}_{\alpha\delta}$



Trace of matrix product:

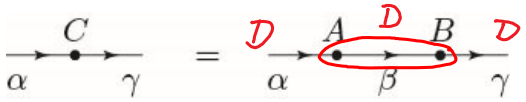
$T = A^\delta{}_\alpha B^\alpha{}_\beta C^\beta{}_\gamma D^\gamma{}_\delta$



Cost of computing contractions

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

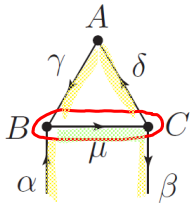
Example 1: cost of matrix multiplication is $\mathcal{O}(D^3)$:



For every fixed α and γ ($D_\alpha \times D_\gamma$ combinations), sum over D_β values of β

Cost = $D_\alpha \cdot D_\gamma \cdot D_\beta$ (simplifies to D^3 if all bond dimensions are = D)

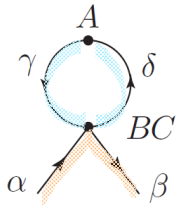
Example 2:



4 legs , 1 sum

$\mathcal{O}(D^4 \cdot D)$

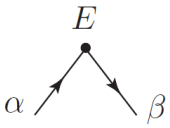
contracting μ



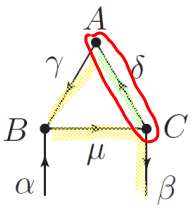
2 legs , 2 sums

$\mathcal{O}(D^2 \cdot D^2)$

contracting $\gamma\delta$



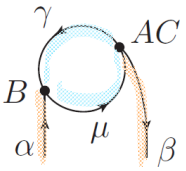
$A^{\delta}{}_{\gamma}{}^{\gamma\alpha}{}_{\mu} B^{\mu}{}_{\beta\delta} C^{\mu}{}_{\beta\delta} = A^{\delta}{}_{\gamma}{}^{\gamma\alpha}{}_{\beta\delta} (BC)^{\beta\delta} = E^{\alpha}{}_{\beta}$



3 legs , 1 sum

$\mathcal{O}(D^3 \cdot D)$

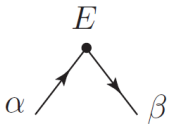
contracting δ



2 legs , 2 sums

$\mathcal{O}(D^2 \cdot D^2)$

contracting $\gamma\mu$



$B^{\gamma\alpha}{}_{\mu} A^{\delta}{}_{\gamma}{}^{\mu}{}_{\beta\delta} C^{\mu}{}_{\beta\delta} = B^{\gamma\alpha}{}_{\mu} (AC)^{\mu}{}_{\beta\gamma} = E^{\alpha}{}_{\beta}$

independent of α !!

First contraction scheme has total cost $\mathcal{O}(D^5)$, second has $\mathcal{O}(D^4)$!!

Finding optimal contraction order is difficult problem! In practice: rely on experience, trial and error…