

Multi-linear Algebra
– Hierarchical Tucker Decomposition –
Lecture 19

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Recall

Recall

- CP decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then

$$\mathbf{A} = \sum_{p=1}^r \bigotimes_{i=1}^d \mathbf{v}_{i,p}$$

Storage of CP format:

CP rank:

Recall

- CP decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then

$$\mathbf{A} = \sum_{p=1}^r \bigotimes_{i=1}^d \mathbf{v}_{i,p}$$

Storage of CP format: $\mathcal{O}(rnd)$

CP rank: minimal r s.t. we can express \mathbf{A} in the above format

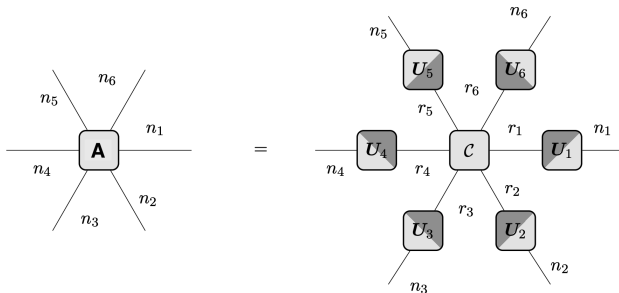
Recall

- Tucker decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then

$$\begin{aligned}\mathbf{A} &= \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathbf{C}[i_1, \dots, i_d] \cdot \mathbf{u}_{1,i_1} \otimes \mathbf{u}_{2,i_2} \otimes \cdots \otimes \mathbf{u}_{d,i_d} \\ &= \mathbf{C} *_1 \mathbf{U}_1 *_2 \mathbf{U}_2 \dots *_d \mathbf{U}_d\end{aligned}$$

Recall

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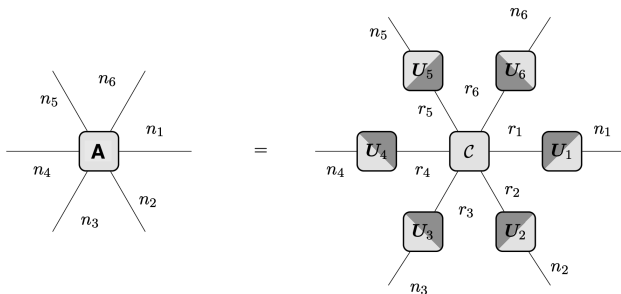


Storage of Tucker format:

T-rank:

Recall

- Tucker decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then



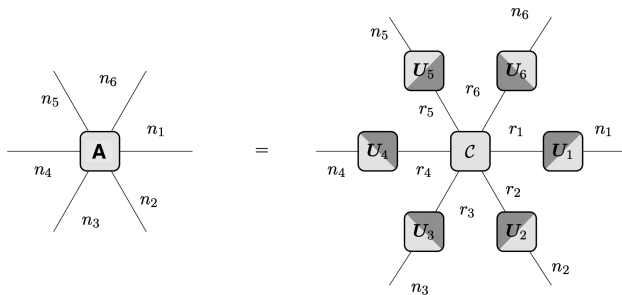
Storage of Tucker format: $\mathcal{O}(r^d + rnd)$

T-rank: $\mathbf{r} = (r_1, \dots, r_d)$

Advantage:

Recall

- Tucker decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then



Storage of Tucker format: $\mathcal{O}(r^d + rnd)$

Advantage:

- 1 Can be computed using HOSVD
- 2 Closed set of low-rank tensors
- 3 Manifold structure on the set of tensors with fixed rank
- 4 Can be sketched

Recall TT format

- TT decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then

$$\begin{aligned}\mathbf{A} &= \mathbf{U}_1 \circ \mathbf{U}_2 \circ \dots \circ \mathbf{U}_d \\ &= \mathbf{U}_1 *_{2,1} \mathbf{U}_2 *_{3,1} \dots *_{3,1} \mathbf{U}_d \\ &= \sum_{k_1=1}^{r_1} \dots \sum_{k_{d-1}=1}^{r_{d-1}} \mathbf{U}_1[:, k_1] \mathbf{U}_2[k_1, :, k_2] \cdots \mathbf{U}_{d-1}[k_{d-2}, :, k_{d-1}] \mathbf{U}_d[k_{d-1}, :]\end{aligned}$$

Recall TT format

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or elementwise

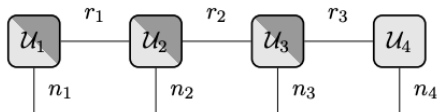
$$\begin{aligned}\mathbf{A}[i_1, \dots, i_d] &= \sum_{k_1=1}^{r_1} \dots \sum_{k_{d-1}=1}^{r_{d-1}} \mathbf{U}_1[i_1, k_1] \mathbf{U}_2[k_1, i_2, k_2] \cdots \mathbf{U}_{d-1}[k_{d-2}, i_{d-1}, k_{d-1}] \mathbf{U}_d[k_{d-1}, i_d]\end{aligned}$$

Recall TT format

- TT decomposition: Let $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$. Then

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or in diagrams



TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d} \\ = \mathbf{A}_{n_2 \dots n_d}^{n_1}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

$$= \mathbf{A}_{n_2 \dots n_d}^{n_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_2 \dots n_d}^{r_1}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

$$= \mathbf{A}_{n_2 \cdots n_d}^{n_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_2 \cdots n_d}^{r_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_3 \cdots n_d}^{r_1 \cdot n_2}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

reshape of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

TT-SVD

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$$= \mathbf{A}_{n_2 \cdots n_d}^{n_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_2 \cdots n_d}^{r_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_3 \cdots n_d}^{r_1 \cdot n_2}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\mathbf{U}_2)_{r_2}^{r_1 \cdot n_2} (\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)_{n_3 \cdots n_d}^{r_2}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

reshape of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

SVD of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

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$$= (\mathbf{U}_1)_{r_1}^{n_1} (\mathbf{U}_2)_{r_2}^{r_1 \cdot n_2} (\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)_{n_4 \dots n_d}^{r_2 \cdot n_3}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

reshape of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

SVD of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

reshape of $(\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)$

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

$$= \mathbf{A}_{n_2 \dots n_d}^{n_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_2 \dots n_d}^{r_1}$$

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$$= (\mathbf{U}_1)_{r_1}^{n_1} (\mathbf{U}_2)_{r_2}^{r_1 \cdot n_2} (\mathbf{U}_3)_{r_3}^{r_2 \cdot n_3} (\boldsymbol{\Sigma}_3 \mathbf{V}_3^\top)_{n_4 \dots n_d}^{r_3}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

reshape of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

SVD of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

reshape of $(\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)$

SVD of $(\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)$

TT-SVD

$$\mathbf{A}_{n_1, \dots, n_d}$$

$$= \mathbf{A}_{n_2 \dots n_d}^{n_1}$$

$$= (\mathbf{U}_1)_{r_1}^{n_1} (\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)_{n_2 \dots n_d}^{r_1}$$

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\vdots

$$= \underbrace{(\mathbf{U}_1)_{r_1}^{n_1}}_{\mathbf{U}_1[n_d]} \cdots \underbrace{(\mathbf{U}_{d-1})_{r_{d-1}}^{r_{d-2} \cdot n_{d-1}}}_{=: \mathbf{U}_{d-1}[n_{d-1}]} \underbrace{(\boldsymbol{\Sigma}_{d-1} \mathbf{V}_{d-1}^\top)_{n_d}^{r_{d-1}}}_{=: \mathbf{U}_d[n_d]}$$

reshape to $n_1 \times \prod_{j \neq i} n_j$

SVD

reshape of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

SVD of $(\boldsymbol{\Sigma}_1 \mathbf{V}_1^\top)$

reshape of $(\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)$

SVD of $(\boldsymbol{\Sigma}_2 \mathbf{V}_2^\top)$

HT decomposition

- Similar idea as TT format:
 - instead of using the nested subspace use a hierarchy of subspaces
- Define a partition tree for the set of mode indices:
 - the root of the tree contains the complete set
 - each leaf contains a single mode index
 - each inner node of the tree contains the union of its children

Tree tensor network

What is a partition tree for the set of mode indices?

Tree tensor network

What is a partition tree for the set of mode indices?

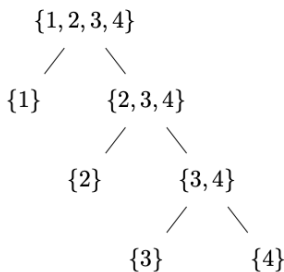
- It is a hierarchical tree
- TT format:

$$\mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$$

$$U_1 \otimes \mathbb{R}^{n_2 \times n_3 \times n_4}$$

$$U_2 \otimes \mathbb{R}^{n_3 \times n_4}$$

$$U_3 \otimes \mathbb{R}^{n_4}$$



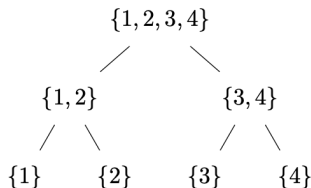
Balanced tree tensor network

- Consider $\mathbf{U} \in \mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$
- Balanced tree of mode indices:

$$\mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4}$$

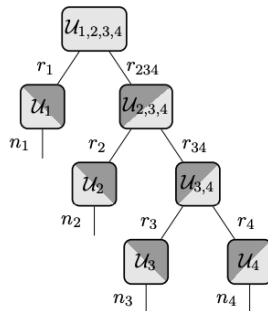
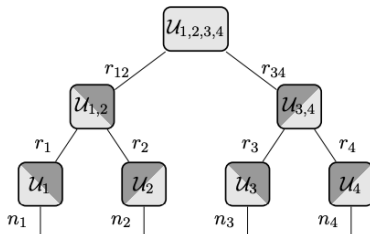
$$\tilde{U}_1 \otimes \tilde{U}_2, \quad \tilde{U}_1 \subseteq \mathbb{R}^{n_1 \times n_2}, \quad \tilde{U}_2 \subseteq \mathbb{R}^{n_3 \times n_4}$$

$$U_1 \otimes U_2 \otimes U_3 \otimes U_4$$



Tree tensor networks in diagrams

- Compare TT vs HT:



Recall matricization

- For a tensor $\mathbf{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$, a collection of dimension indices $t \subset \{1, \dots, d\}$, and its complement $s = \{1, \dots, d\} \setminus t$, we define

$$\mathbf{A}^{(t)} \in \mathbb{R}^{n_t \times n_s}, \quad n_t = \prod_{k \in t} n_k, \quad n_s = \prod_{k \in s} n_k$$

elementwise defined as

$$[\mathbf{A}^{(t)}]_{(i_k)_{k \in t}, (i_\ell)_{\ell \in s}} = \mathbf{A}_{i_1, \dots, i_d}$$

Matricization example

Consider

$$\mathbf{A}_{i_1, i_2, i_3, i_4} = i_1 + 2(i_1 - 1) + 4(i_3 - 1) + 8(i_4 - 1), \quad i_1, i_2, i_3, i_4 \in \{1, 2\}$$

We chose the lexicographical ordering for compound indices

$$(i_p, \dots, i_q) \mapsto \ell = i_p + n_p(i_{p+1} - 1) + n_p n_{p+1}(i_{p+2} - 1) + \dots + i_q n_p \cdots n_{q-1}$$

Compute

$$\mathbf{A}^{\{\{1\}\}} =$$

Matricization example

Consider

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Compute

$$\mathbf{A}^{\{\{1\}\}} = \begin{bmatrix} 1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 \end{bmatrix}$$

Matricization example

Consider

$$\mathbf{A}_{i_1, i_2, i_3, i_4} = i_1 + 2(i_1 - 1) + 4(i_3 - 1) + 8(i_4 - 1), \quad i_1, i_2, i_3, i_4 \in \{1, 2\}$$

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Compute

$$\mathbf{A}^{\{\{3\}\}} =$$

Matricization example

Consider

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Compute

$$\mathbf{A}^{\{\{3\}\}} = \begin{bmatrix} 1 & 2 & 3 & 4 & 9 & 10 & 11 & 12 \\ 5 & 6 & 7 & 8 & 13 & 14 & 15 & 16 \end{bmatrix}$$

Matricization example

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Compute

$$\mathbf{A}^{(\{2,3,4\})} =$$

Matricization example

Consider

$$\mathbf{A}_{i_1, i_2, i_3, i_4} = i_1 + 2(i_1 - 1) + 4(i_3 - 1) + 8(i_4 - 1), \quad i_1, i_2, i_3, i_4 \in \{1, 2\}$$

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Compute

$$\mathbf{A}^{(\{2,3,4\})} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ 7 & 8 \\ 9 & 10 \\ 11 & 12 \\ 13 & 14 \\ 15 & 16 \end{bmatrix} = (\mathbf{A}^{(\{1\})})^\top$$

Matricization Tucker format

Consider the tensor

$$\mathbf{A} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} \otimes \begin{bmatrix} 5 \\ 6 \end{bmatrix}$$

Matricization Tucker format

Consider the tensor

$$\mathbf{A} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} \otimes \begin{bmatrix} 5 \\ 6 \end{bmatrix} = \left[\begin{bmatrix} 15 & 20 \\ 30 & 40 \end{bmatrix}, \begin{bmatrix} 18 & 24 \\ 36 & 48 \end{bmatrix} \right]$$

Then its $(\{1, 2\})$ -matricization is

$$\mathbf{A}^{(\{1,2\})}$$

Matricization Tucker format

Consider the tensor

$$\mathbf{A} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} \otimes \begin{bmatrix} 5 \\ 6 \end{bmatrix} = \left[\begin{bmatrix} 15 & 20 \\ 30 & 40 \end{bmatrix}, \begin{bmatrix} 18 & 24 \\ 36 & 48 \end{bmatrix} \right]$$

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Then its $(\{1, 2\})$ -matricization is

$$\mathbf{A}^{(\{1,2\})} = \begin{bmatrix} 15 & 18 \\ 30 & 36 \\ 20 & 24 \\ 40 & 48 \end{bmatrix} = \left(\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} \right)^{(\{1,2\})} \cdot \left(\left(\begin{bmatrix} 5 \\ 6 \end{bmatrix} \right)^{(\{1\})} \right)^{\top}$$

Matricization Tucker format

Consider the tensor $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$

$$\mathbf{A} = \sum_{j_1=1}^{k_1} \sum_{j_2=1}^{k_2} \sum_{j_3=1}^{k_3} c_{j_1, j_2, j_3} \mathbf{u}_{j_1, 1} \otimes \mathbf{u}_{j_2, 2} \otimes \mathbf{u}_{j_3, 3}$$

Then

$$\mathbf{A}^{(\{1,2\})} = \sum_{j_1=1}^{k_1} \sum_{j_2=1}^{k_2} (\mathbf{u}_{j_1, 1} \otimes \mathbf{u}_{j_2, 2})^{(\{1,2\})} \cdot \left(\sum_{j_3=1}^{k_3} c_{j_1, j_2, j_3} \mathbf{u}_{j_3, 3} \right)^{\top}$$

Matricization Tucker format

Consider the tensor $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$

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Then

$$\mathbf{A}^{(\{1,2\})} = \sum_{j_1=1}^{k_1} \sum_{j_2=1}^{k_2} (\mathbf{u}_{j_1, 1} \otimes \mathbf{u}_{j_2, 2})^{(\{1,2\})} \cdot \left(\sum_{j_3=1}^{k_3} c_{j_1, j_2, j_3} \mathbf{u}_{j_3, 3} \right)^{\top}$$

Rank bound

Lemma:

Let $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ with

$$\mathbf{A} = \sum_{j_1=1}^{k_1} \sum_{j_2=1}^{k_2} \sum_{j_3=1}^{k_3} c_{j_1, j_2, j_3} \mathbf{u}_{j_1, 1} \otimes \mathbf{u}_{j_2, 2} \otimes \mathbf{u}_{j_3, 3}.$$

Then

$$\text{rank}(\mathbf{A}^{\{1,2\}}) \leq \min(\{k_1 \cdot k_2, k_3\}).$$

Root-to-leaves truncated hierarchical SVD¹

Set $\mathcal{I} = n_1 \times \dots \times n_d$, and let $T_{\mathcal{I}}$ be a dimension tree of depth $p \in \mathbb{N}$. We call $\mathcal{L}(T_{\mathcal{I}})$ the leafs of the $T_{\mathcal{I}}$, and $\mathcal{I}(T_{\mathcal{I}})$ are the internal nodes of the $T_{\mathcal{I}}$.

Algorithm:

Input: $\mathbf{A} \in \mathbb{R}^{\mathcal{I}}$, $T_{\mathcal{I}}$, target rank $(r_t)_{t \in T_{\mathcal{I}}}$

Output: $(\mathbf{U}_t)_{t \in \mathcal{L}(T_{\mathcal{I}})}$, $(\mathbf{B}_t)_{t \in \mathcal{I}(T_{\mathcal{I}})}$

for $t \in \mathcal{L}(T_{\mathcal{I}})$

$$\mathbf{U}_t, \mathbf{\Sigma}_t, \mathbf{V}_t = \text{SVD}(\mathbf{A}^{(t)}, r_t)$$

for $\ell = p - 1 : 0$

for $t \in \mathcal{I}(T_{\mathcal{I}})$ on level ℓ

$$\mathbf{U}_t, \mathbf{\Sigma}_t, \mathbf{V}_t = \text{SVD}(\mathbf{A}^{(t)}, r_t)$$

\mathbf{U}_{t_1} and \mathbf{U}_{t_2} be successors of t .

$$\text{compute } (\mathbf{B}_t)_{i,j,k} = \langle (\mathbf{U}_{t_1})_i, (\mathbf{U}_{t_2})_j \otimes (\mathbf{U}_{t_1})_k \rangle$$

Compute $(\mathbf{B}_{\{1,\dots,d\}})_{1,j,k} = \langle (\mathbf{A}, (\mathbf{U}_{t_1})_j \otimes (\mathbf{U}_{t_2})_k) \rangle$

¹Grasedyck, SIAM Journal on Matrix Analysis and Applications, 2010

Hierarcical Tucker format

Tree tensor network:

$$(\mathbf{U}_t)_{t \in \mathcal{L}(T_{\mathcal{I}})} \quad \text{and} \quad (\mathbf{B}_t)_{t \in \mathcal{I}(T_{\mathcal{I}})}$$

Storage:

Hierarcical Tucker format

Tree tensor network:

$$(\mathbf{U}_t)_{t \in \mathcal{L}(T_{\mathcal{I}})} \quad \text{and} \quad (\mathbf{B}_t)_{t \in \mathcal{I}(T_{\mathcal{I}})}$$

Storage: $\mathcal{O}(rnd + dr^3)$

Compare to TT: $\mathcal{O}(dnr^2)$

Why HT?

Hierarcical Tucker format

Tree tensor network:

$$(\mathbf{U}_t)_{t \in \mathcal{L}(T_{\mathcal{I}})} \quad \text{and} \quad (\mathbf{B}_t)_{t \in \mathcal{I}(T_{\mathcal{I}})}$$

Storage: $\mathcal{O}(rnd + dr^3)$

Compare to TT: $\mathcal{O}(dnr^2)$

Why HT?

\Rightarrow Remember, the tensor rank is not uniquely defined!

A tensor \mathbf{A} may be *exactly* represented in HT and TT format, however, the ranks appearing in HT can be lower!
(Consequence of general rank bounds²)

²Grasedyck & Hackbusch, Computational Methods in Applied Mathematics, 2011