# A Matlab toolbox for tensors in hierarchical Tucker format

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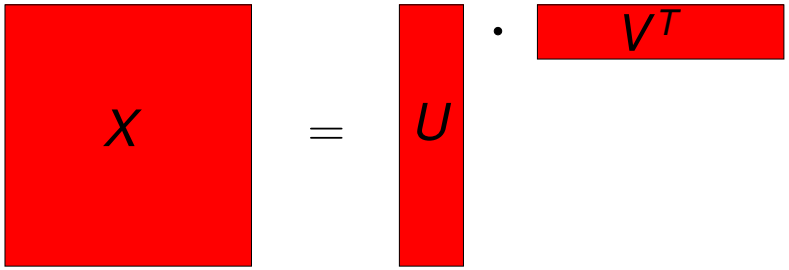
# Motivation

Low-rank matrix:




- Reduced storage cost: $O(n_1 r + n_2 r)$ instead of $O(n_1 n_2)$
- Basic operations (addition, multiplication by a matrix) possible
- Best lower-rank approximation by truncated SVD

We define a tensor as an array $\mathcal{X} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$

Goal:

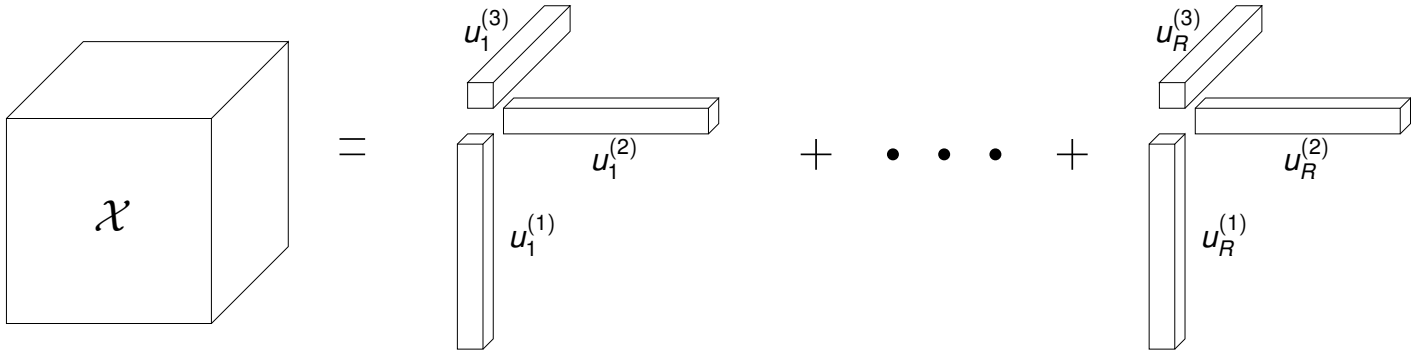
- Concept of low-rank tensor, similar to that of low-rank matrix
- Storage cost linearly dependent on $d$

# Contents

# CP and Tucker formats

# CP format

$$\mathrm{vec}(\mathcal{X}) = \sum_{j=1}^{R} u_j^{(d)} \otimes \cdots \otimes u_j^{(1)}, \quad u_j^{(\mu)} \in \mathbb{R}^{n_\mu}.$$



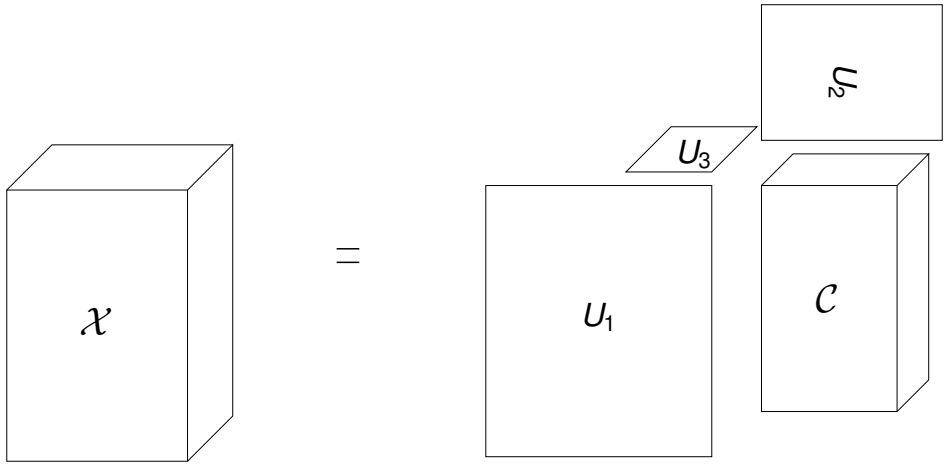

**Pro and Contra**

- \+ Storage requirements linear in d: $dnR$
- – Approximation in CP format cumbersome

# Tucker format

$$\mathrm{vec}(\mathcal{X}) = \sum_{j_1=1}^{r_1} \cdots \sum_{j_d=1}^{r_d} \mathcal{C}_{j_1,\ldots,j_d} u_{j_d}^{(d)} \otimes \cdots \otimes u_{j_1}^{(1)} = (U_d \otimes \cdots \otimes U_1)\mathrm{vec}(\mathcal{C}),$$

with $\mathcal{C} \in \mathbb{R}^{r_1 \times \cdots \times r_d}$, $U_\mu = [u_1^{(\mu)}, \ldots, u_{r_\mu}^{(\mu)}] \in \mathbb{R}^{n_\mu \times r_\mu}$.




**Pro and Contra**

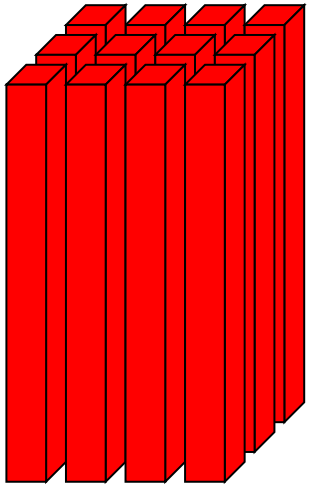
+ Efficient quasi-best approximation in Tucker format (HOSVD)
− Storage requirements exponential in d: $dnr + r^d$

# Hierarchical Tucker format

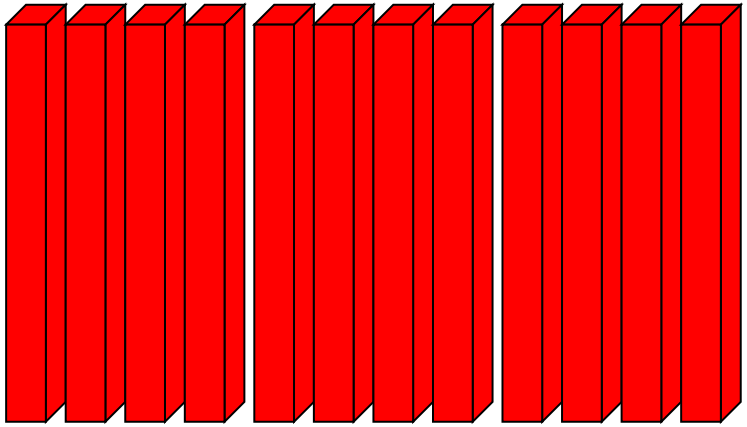

- L. Grasedyck. Hierarchical singular value decomposition of tensors. *SIAM J. Matrix Anal. Appl.*, 31(4):2029–2054, 2010.
- W. Hackbusch and S. Kühn. A new scheme for the tensor representation. *J. Fourier Anal. Appl.*, 15(5):706–722, 2009.

# Matricization

1-mode matricization:



$\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$



$X^{(1)} \in \mathbb{R}^{n_1 \times (n_2 n_3 \cdots n_d)}$

$\mu$-mode matricization:

$$X^{(\mu)} \in \mathbb{R}^{n_\mu \times (n_1 \cdots n_{\mu-1} n_{\mu+1} \cdots n_d)}, \qquad \mu = 1, \ldots, d.$$

General matricization for mode decomposition $\{1, \ldots, d\} = t \cup s$:

$$X^{(t)} \in \mathbb{R}^{(n_{t_1} \cdots n_{t_k}) \times (n_{s_1} \cdots n_{s_{d-k}})} \quad \text{with} \quad \left(X^{(t)}\right)_{(i_{t_1}, \ldots, i_{t_k}), (i_{s_1}, \ldots, i_{s_{d-k}})} := \mathcal{X}_{i_1, \ldots, i_d}.$$

# Hierarchical construction

**Definition** of $\mathcal{H}$-Tucker rank-$(r_t)_{t\in\mathcal{T}}$ tensor:

$$\mathcal{H}-\text{Tucker}(r_t)_{t\in\mathcal{T}} = \left\{\mathcal{X}\in\mathbb{R}^{n_1\times\cdots\times n_d} : rank(X^{(t)}) \le r_t \quad \forall t\in\mathcal{T}\right\}$$

Singular value decomposition: $X^{(t)} = U_t\Sigma_t U_s^T$.

Column spaces are nested $\rightsquigarrow$

$$\begin{aligned} t = t_1 \dot\cup t_2 \quad &\Rightarrow \quad \text{span}(U_t) \subset \text{span}(U_{t_2}\otimes U_{t_1}) \\ &\Rightarrow \quad \exists B_t : \; U_t = (U_{t_2}\otimes U_{t_1})B_t. \end{aligned}$$

Size of $U_t$:

$$U_t \in \mathbb{R}^{n_{t_1}\cdots n_{t_k}\times r_t} \quad \text{with} \quad r_t = \text{rank}\big(X^{(t)}\big).$$

Size of $B_t$:

$$B_t \in \mathbb{R}^{r_{t_1} r_{t_2}\times r_t} \quad \text{with} \quad r_t = \text{rank}\big(X^{(t)}\big).$$

# Hierarchical construction

Singular value decomposition: $X^{(t)} = U_t \Sigma_t U_s^T$.

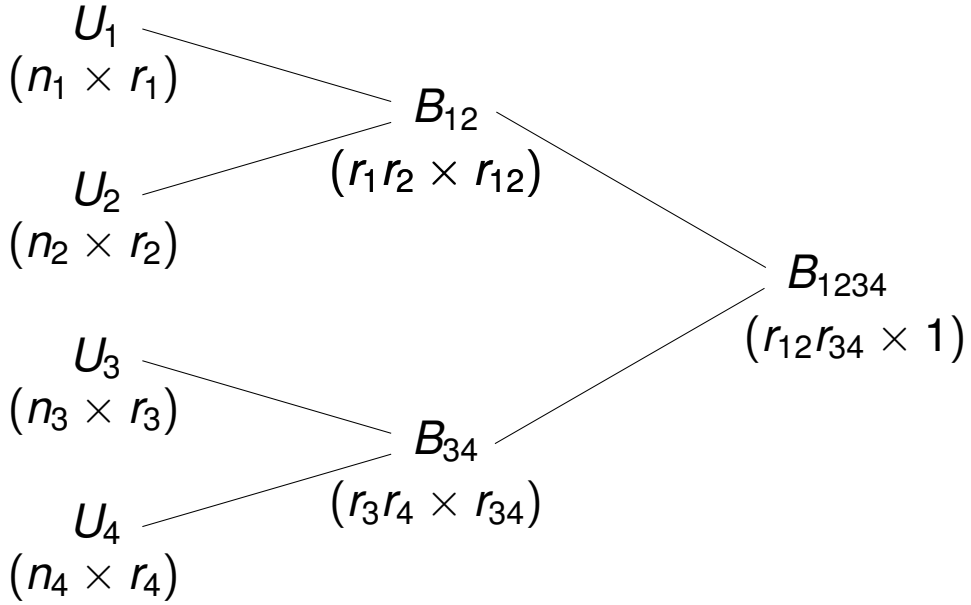
$$\begin{aligned} t = t_1 \dot{\cup} t_2 \quad &\Rightarrow \quad \mathrm{span}(U_t) \subset \mathrm{span}(U_{t_2} \otimes U_{t_1}) \\ &\Rightarrow \quad \exists B_t : \; U_t = (U_{t_2} \otimes U_{t_1}) B_t. \end{aligned}$$

For $d = 4$:

$$\begin{aligned} U_{12} &= (U_2 \otimes U_1) B_{12} \\ U_{34} &= (U_4 \otimes U_3) B_{34} \\ \mathrm{vec}(\mathcal{X}) = X^{(1234)} &= (U_{34} \otimes U_{12}) B_{1234} \\ \Rightarrow \quad \mathrm{vec}(\mathcal{X}) &= (U_4 \otimes U_3 \otimes U_2 \otimes U_1)(B_{34} \otimes B_{12}) B_{1234}. \end{aligned}$$

# Dimension tree

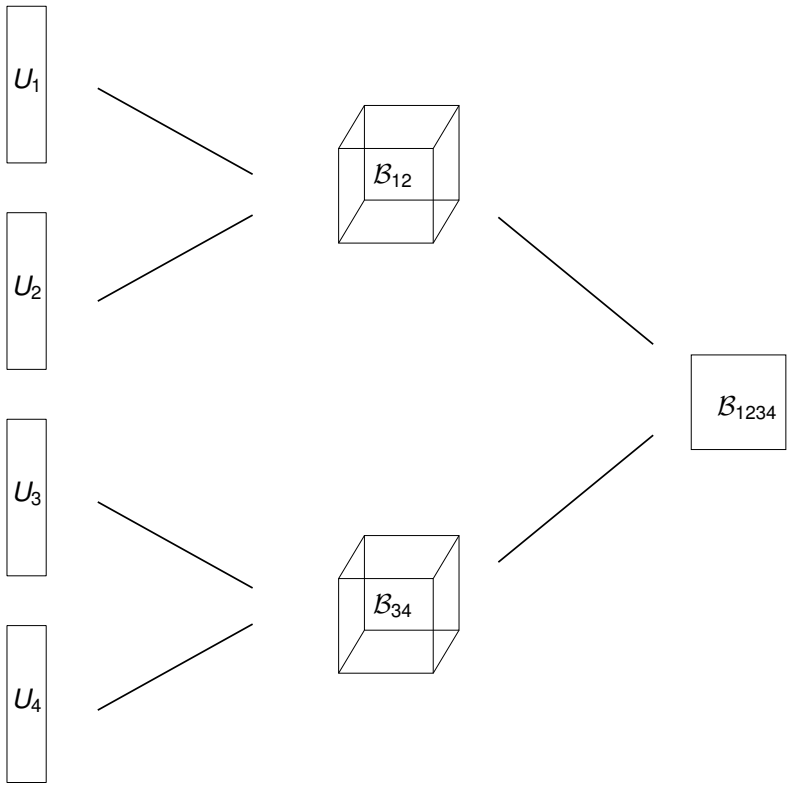
Tree structure for $d = 4$:




Reshape:

$$
\begin{aligned}
B_{12} \in \mathbb{R}^{r_1 r_2 \times r_{12}} \quad &\Rightarrow \quad \mathcal{B}_{12} \in \mathbb{R}^{r_1 \times r_2 \times r_{12}} \\
B_{34} \in \mathbb{R}^{r_3 r_4 \times r_{34}} \quad &\Rightarrow \quad \mathcal{B}_{34} \in \mathbb{R}^{r_3 \times r_4 \times r_{34}} \\
B_{1234} \in \mathbb{R}^{r_{12} r_{34} \times 1} \quad &\Rightarrow \quad \mathcal{B}_{1234} \in \mathbb{R}^{r_{12} \times r_{34}}
\end{aligned}
$$

# Dimension tree




Storage requirements for general $d$:

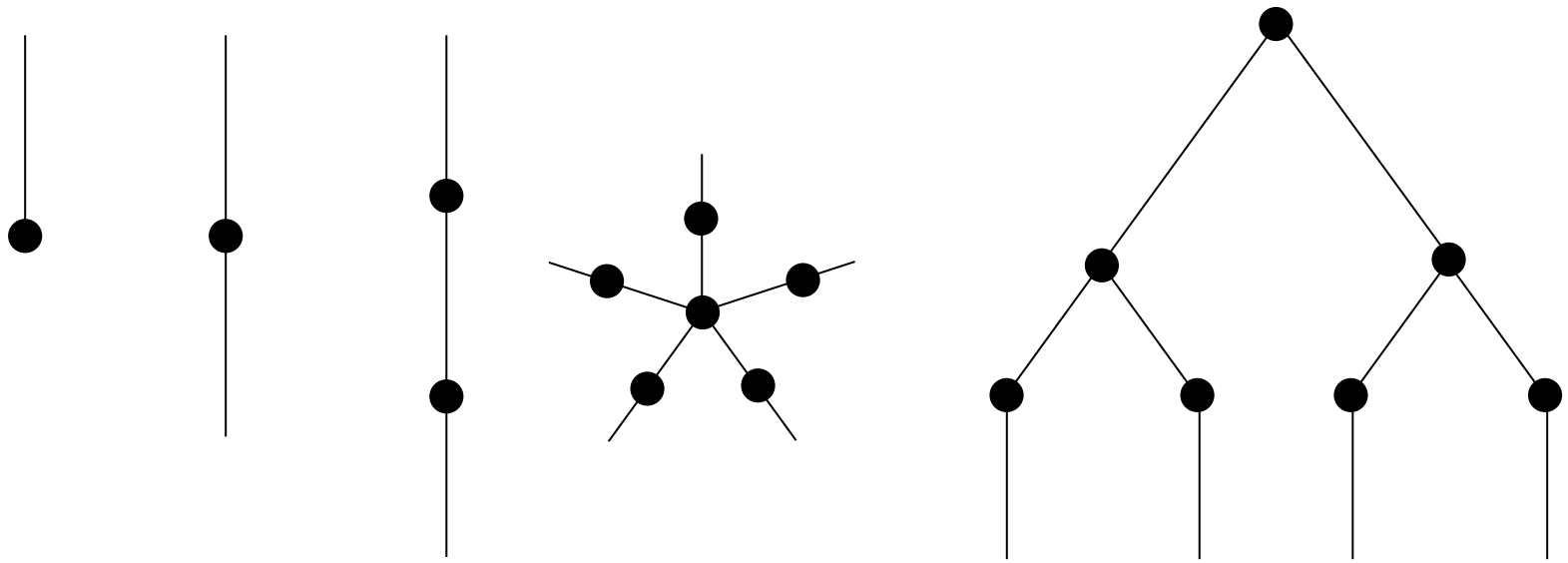
$$\mathcal{O}(dnr) + \mathcal{O}(dr^3),$$

where $r = max\{r_t\}$, $n = \max\{n_\mu\}$.

# Tensor network notation

Tensor network: Collection of tensors connected by tensor contractions.

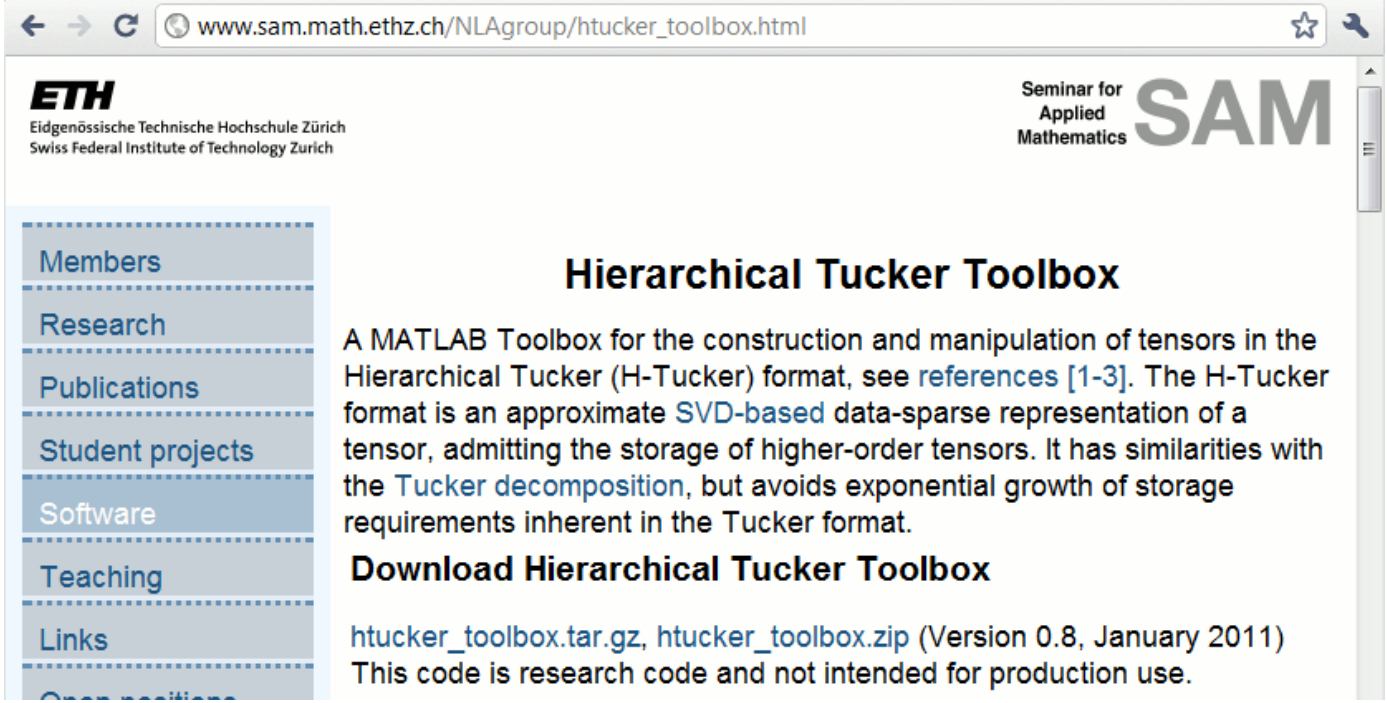
Examples:



# MATLAB `htucker` toolbox

# MATLAB htucker toolbox

www.sam.math.ethz.ch/NLAgroup/htucker_toolbox.html




- `htucker` provides MATLAB class for storing and manipulating tensor in low-rank format.
- Several operations overloaded (`+ - .* norm` ...)
- Set of frequently used utilities.
- Main goal: Painless experimentation with algorithms.

# Existing MATLAB Toolboxes

- MATLAB Tensor Toolbox by T. Kolda and B. Bader
  `csmr.ca.sandia.gov/~tgkolda/TensorToolbox`

- TT Toolbox by I. Oseledets
  `spring.inm.ras.ru/osel/?p=31`

# Basic functionality for MATLAB class `htensor`

`x = htenones([4 5 6 7])` constructs `htensor` of size $4 \times 5 \times 6 \times 7$, with all entries one.

`x = htenrandn([4 5 6 7])` constructs `htensor` of size $4 \times 5 \times 6 \times 7$, with random ranks and random entries.

`x(1, 3, 4, 2)` returns entry of $\mathcal{X}$.

`x(1, 3, :, :)` returns slice of $\mathcal{X}$ as an `htensor`.

`full(x)` returns full tensor represented by $\mathcal{X}$. (use with care)

`spy(x)` displays spy plots of $U_t$, $B_t$, on the dimension tree.

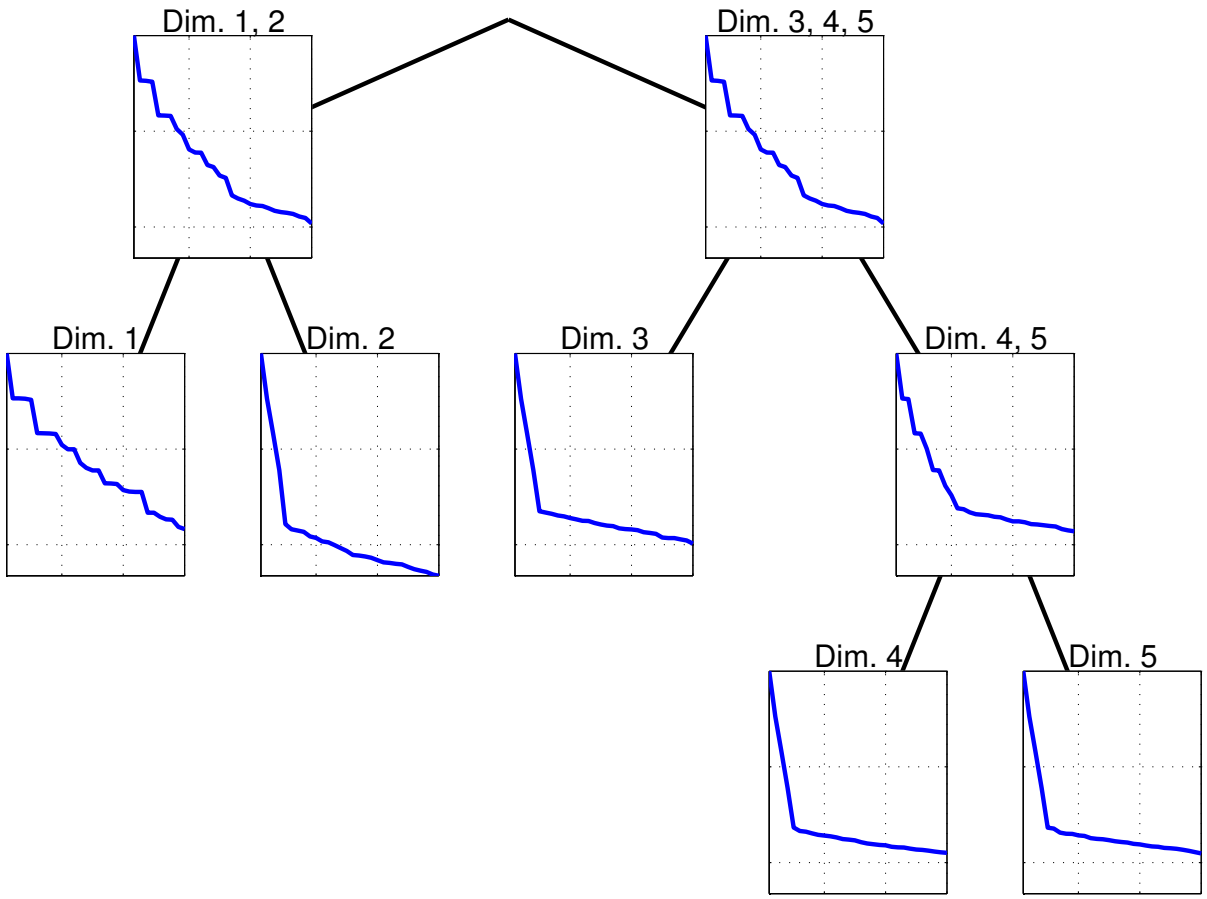
`disp_tree(x)` returns tree structure/ranks:

```
ans is an htensor of size 4 x 5 x 6 x 7
  1-4      1; 6 3 1
  1-2      2; 3 4 6
    1      4; 4 3
    2      5; 5 4
  3-4      3; 3 3 3
    3      6; 6 3
    4      7; 7 3
```

# Singular value tree

`plot_sv`(x) plots singular values of corresponding matricizations in the dimension tree of a tensor $\mathcal{X}$.

Example: Singular value tree of an order 5 tensor.



# Basic operations

- Matrix $\times$ tensor
- Addition
- Inner product

# Matrix $\times$ tensor

Application of matrix $A \in \mathbb{R}^{m \times n_\mu}$ to mode $\mu$ of $\mathcal{X} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$:

$$\mathcal{Y} = A \circ_\mu \mathcal{X} \quad \Leftrightarrow \quad Y^{(\mu)} = AX^{(\mu)}.$$

Nearly trivial if $\mathcal{X}$ is in $\mathcal{H}$-Tucker format:

$$\begin{aligned} A \circ_\mu \mathcal{X} &= A \circ_\mu \big((U_1, \ldots, U_d) \circ \mathcal{C}\big) \\ &= (U_1, \ldots, U_{\mu-1}, AU_\mu, U_{\mu+1}, \ldots, U_d) \circ \mathcal{C} \end{aligned}$$

- Almost no operations required.
- Ranks stay the same.
- Orthogonality destroyed.

`ttm(x, A, 2)` applies matrix $A$ to `htensor` $\mathcal{X}$ in mode 2.
`y = ttm(x, {A, B, C}, [2, 3, 4])`
`y = ttm(x, @(x)(fft(x)), 2)` applies FFT in mode 2.

# Addition of low-rank matrices

Addition of two matrices in low-rank format:

$$A = U_1 \Sigma_A U_2^T, \qquad B = V_1 \Sigma_B V_2^T$$

$\Rightarrow$

$$A + B = \begin{bmatrix} U_1 & V_1 \end{bmatrix} \begin{bmatrix} \Sigma_A & 0 \\ 0 & \Sigma_B \end{bmatrix} \begin{bmatrix} U_2 & V_2 \end{bmatrix}^T$$

- No operations required.
- Rank increases.
- Orthogonality destroyed.

# Addition of low-rank tensors

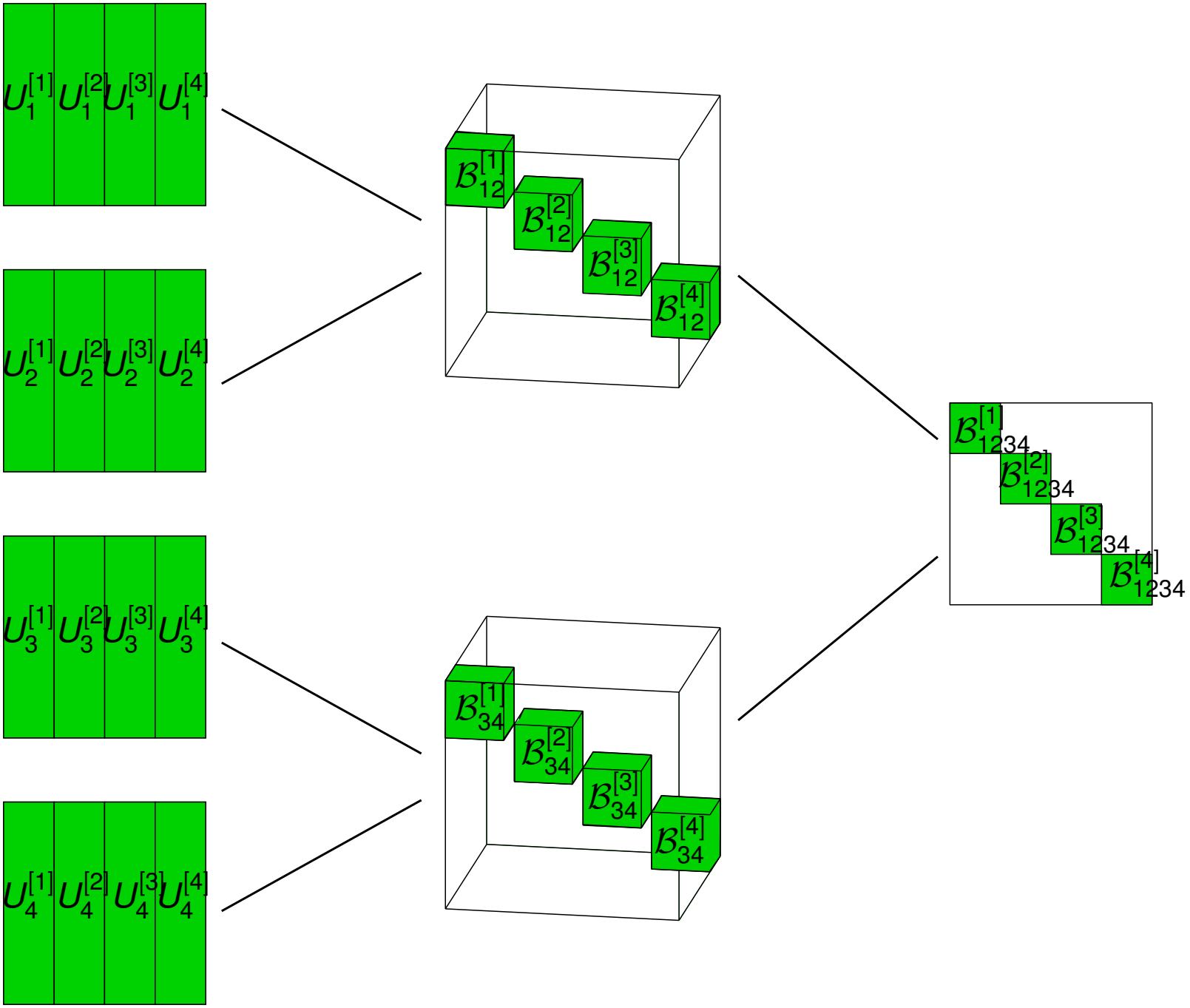
Addition of four tensors $\mathcal{X}_1, \mathcal{X}_2, \mathcal{X}_3, \mathcal{X}_4$ in $\mathcal{H}$-Tucker format:

$$\mathcal{X}_1 + \mathcal{X}_2 + \mathcal{X}_3 + \mathcal{X}_4.$$

Proceed as in matrix case by embedding factors in larger matrices.

- No operations required.
- $\mathcal{H}$-Tucker rank increases.
- Orthogonality destroyed.

Command in `htucker`: `x1 + x2 + x3 + x4`


$U_1^{[1]}$ $U_1^{[2]}$ $U_1^{[3]}$ $U_1^{[4]}$
$U_2^{[1]}$ $U_2^{[2]}$ $U_2^{[3]}$ $U_2^{[4]}$
$U_3^{[1]}$ $U_3^{[2]}$ $U_3^{[3]}$ $U_3^{[4]}$
$U_4^{[1]}$ $U_4^{[2]}$ $U_4^{[3]}$ $U_4^{[4]}$
$\mathcal{B}_{12}^{[1]}$ $\mathcal{B}_{12}^{[2]}$ $\mathcal{B}_{12}^{[3]}$ $\mathcal{B}_{12}^{[4]}$
$\mathcal{B}_{34}^{[1]}$ $\mathcal{B}_{34}^{[2]}$ $\mathcal{B}_{34}^{[3]}$ $\mathcal{B}_{34}^{[4]}$
$\mathcal{B}_{1234}^{[1]}$ $\mathcal{B}_{1234}^{[2]}$ $\mathcal{B}_{1234}^{[3]}$ $\mathcal{B}_{1234}^{[4]}$

# Orthogonalization

Any tensor $\mathcal{X}$ in $\mathcal{H}$-Tucker format can be orthogonalized in the sense that all factors in the dimension tree, except for the root node, contain orthonormal columns, $U_t^T U_t = I$.

Example: $\mathrm{vec}(\mathcal{X}) = (U_4 \otimes U_3 \otimes U_2 \otimes U_1)(B_{34} \otimes B_{12})B_{1234}$.

Step 1: QR decompositions $U_t = Q_t R_t \rightsquigarrow$

$$\mathrm{vec}(\mathcal{X}) = (Q_4 \otimes Q_3 \otimes Q_2 \otimes Q_1)(\widetilde{B}_{34} \otimes \widetilde{B}_{12})B_{1234}$$

with $\widetilde{B}_{34} := (R_4 \otimes R_3)B_{34}$, $\widetilde{B}_{12} := (R_2 \otimes R_1)B_{12}$.

Step 2: QR decompositions $\widetilde{B}_{34} = Q_{34}R_{34}$, $\widetilde{B}_{12} = Q_{12}R_{12} \rightsquigarrow$

$$\mathrm{vec}(\mathcal{X}) = (Q_4 \otimes Q_3 \otimes Q_2 \otimes Q_1)(Q_{34} \otimes Q_{12})\widetilde{B}_{1234}$$

with $\widetilde{B}_{1234} := (R_{34} \otimes R_{12})B_{1234}$.

Compt. requirements for general $d$: $\mathcal{O}(dnr^2) + \mathcal{O}(dr^4)$.

Command in `htucker`: `x = orthog(x)`

# Inner product

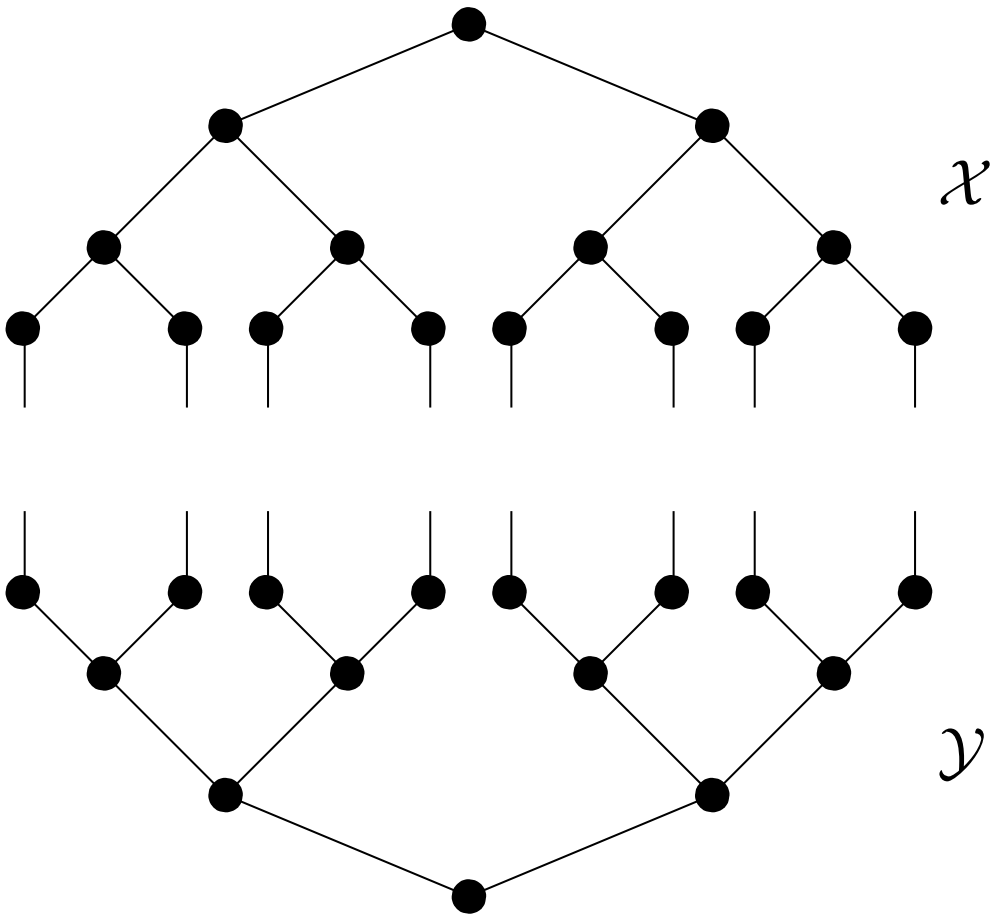
Inner product of two tensors $\mathcal{X}, \mathcal{Y} \in \mathbb{R}^{n_1 \times \cdots n_d}$:

$$\langle \mathcal{X}, \mathcal{Y} \rangle = \langle \mathrm{vec}(\mathcal{X}), \mathrm{vec}(\mathcal{Y}) \rangle = \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} x_{i_1,\ldots,i_d} y_{i_1,\ldots,i_d}.$$

Can be performed efficiently in $\mathcal{H}$-Tucker, provided that $\mathcal{X}, \mathcal{Y}$ have compatible dimension trees.

- `htucker` command: `innerprod(x,y)`
- Overall cost: $\mathcal{O}(dnr^2) + \mathcal{O}(dr^4)$.

# Computation of inner product




$$\langle \mathcal{X}, \mathcal{Y} \rangle = \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} x_{i_1,\ldots,i_d} y_{i_1,\ldots,i_d}.$$

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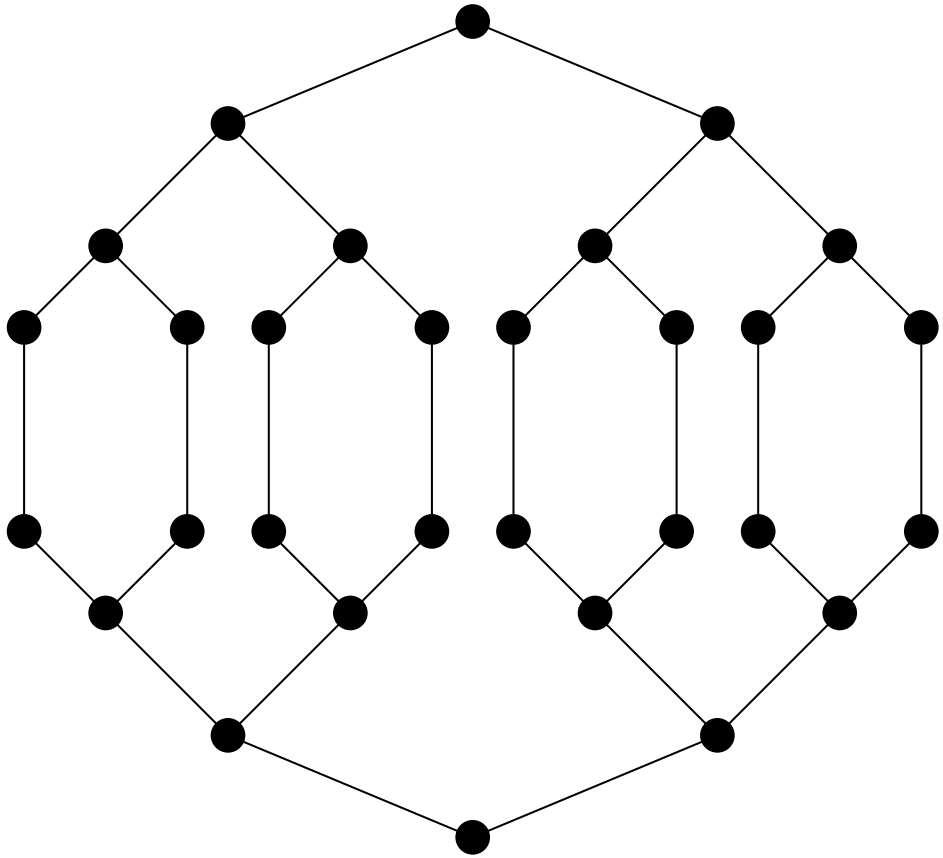

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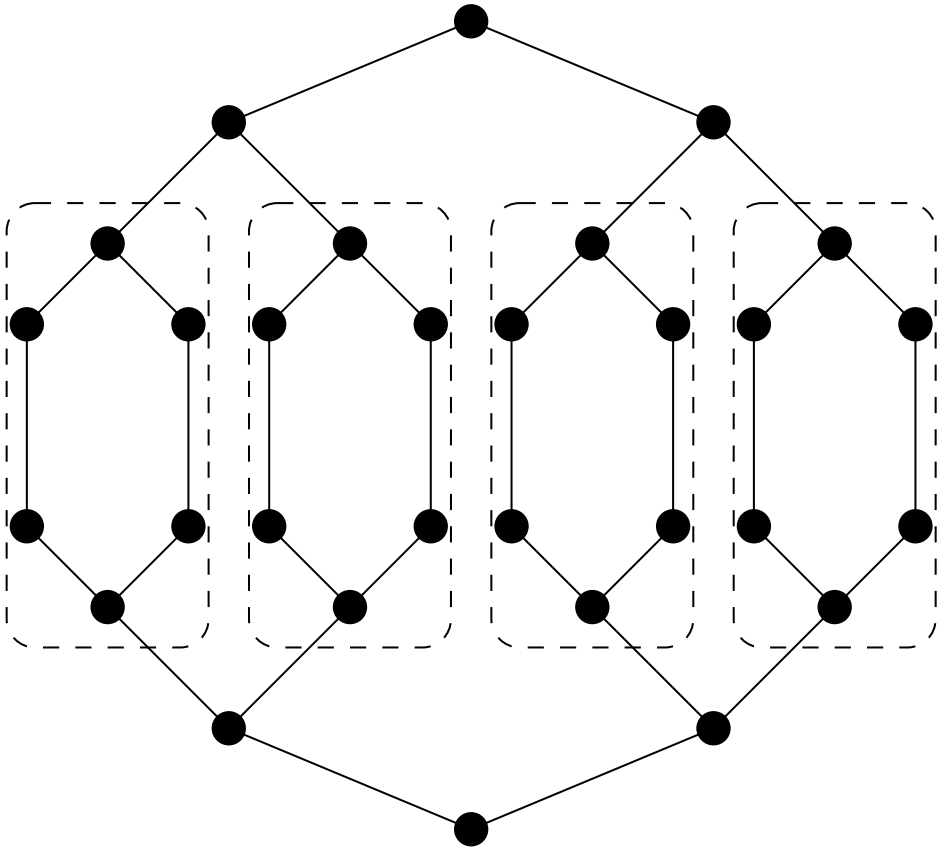

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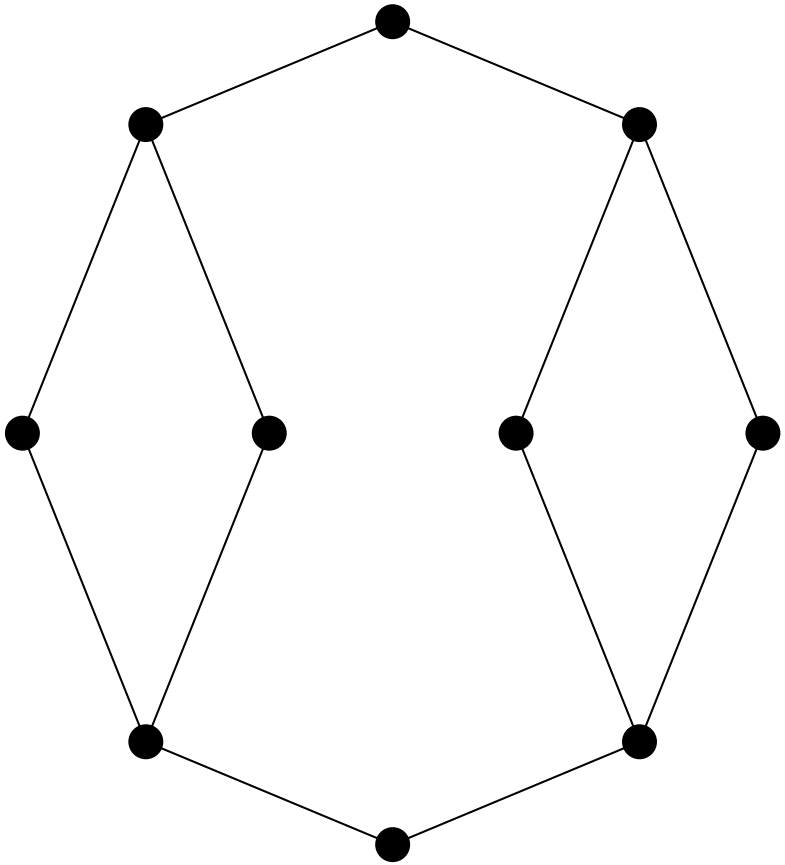

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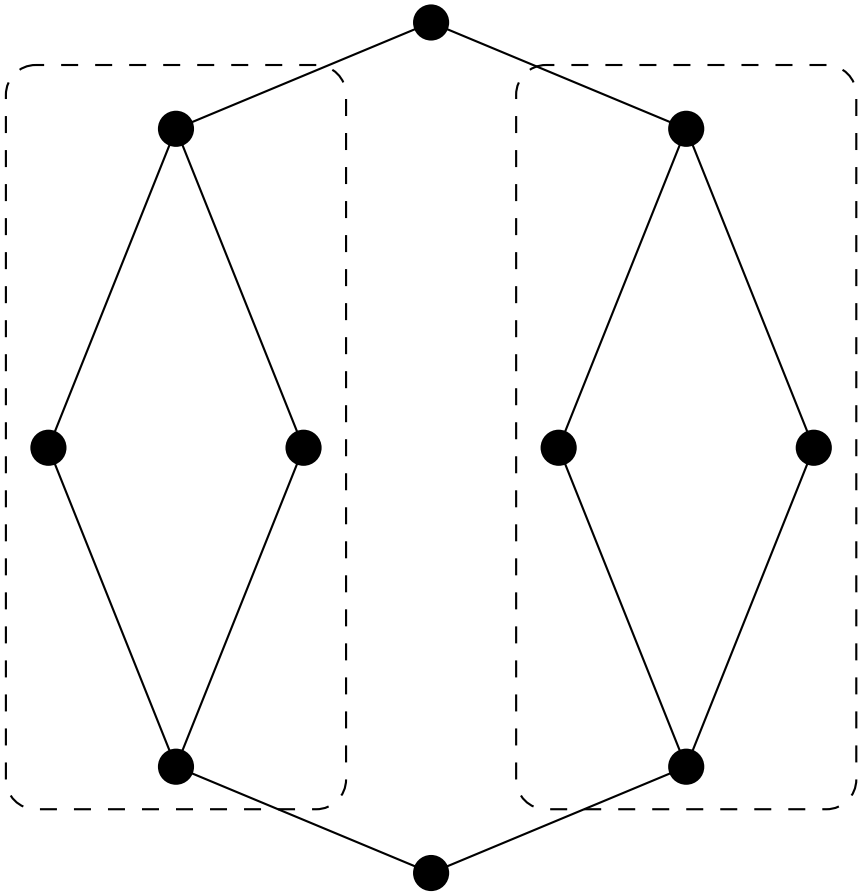

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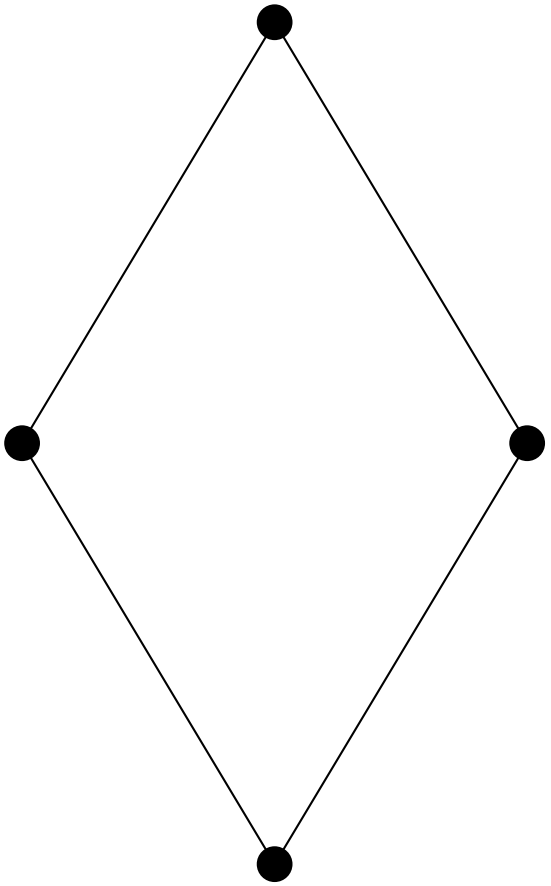

# Advanced operations

- Truncation of explicitly given tensor
- Truncation of $\mathcal{H}$-Tucker tensor

# Truncation of explicit tensor

Let $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ be explicitly given.

- For each tree node $t$, let $W_t$ contain the $r_t$ dominant left singular vectors of $X^{(t)}$ and define projection

$$\pi_t \mathcal{X} = W_t W_t^H \circ_t \mathcal{X} \qquad \Leftrightarrow \qquad \pi_t X^{(t)} = W_t W_t^H X^{(t)}.$$

- Truncated tensor:

$$\tilde{\mathcal{X}} := \Big(\prod_{t \in \mathcal{T}_L} \pi_t\Big) \cdots \Big(\prod_{t \in \mathcal{T}_1} \pi_t\Big) \mathcal{X},$$

  where $\mathcal{T}_\ell$ contains all nodes on level $\ell$.
- [Grasedyck'2010]: $\|\mathcal{X} - \tilde{\mathcal{X}}\| \leq \sqrt{2d-3}\, \|\mathcal{X} - \mathcal{X}_{\text{best}}\|$.

# Truncation of explicit tensor

Example:

$$\begin{aligned}\mathrm{vec}\tilde{\mathcal{X}} &= (W_4 W_4^H \otimes W_3 W_3^H \otimes W_2 W_2^H \otimes W_1 W_1^H)(W_{34} W_{34}^H \otimes W_{12} W_{12}^H)\mathrm{vec}\mathcal{X} \\ &= (W_4 \otimes W_3 \otimes W_2 \otimes W_1) \cdots \\ &\quad (\underbrace{[W_4^H \otimes W_3^H] W_{34}}_{=:B_{34}} \otimes \underbrace{[W_2^H \otimes W_1^H] W_{12}}_{=:B_{12}}) \underbrace{([W_{34}^H \otimes W_{12}^H]\mathrm{vec}\mathcal{X})}_{=:B_{1234}}.\end{aligned}$$

`opts.max_rank = 10` maximal rank at truncation.
`opts.rel_eps = 1e-6` maximal relative truncation error.
`opts.abs_eps = 1e-6` maximal absolute truncation error.
Condition `max_rank` takes precedence over `rel_eps` and `abs_eps`.
`xt = htensor.truncate_rtl(x, opts)` returns truncated tensor $\tilde{\mathcal{X}}$ of a multidimensional array.

Remark: There is also a significantly faster `htensor.truncate_ltr` (proceeds successively from leafs to roots), for which the same error bound holds [Tobler'10].

# Truncation of $\mathcal{H}$-Tucker tensor

Let $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ be in $\mathcal{H}$-Tucker format and *orthogonalized*.

- Compute left singular vectors of $X^{(t)} = U_t V_t^T$ from eigenvectors of

$$X^{(t)} \left(X^{(t)}\right)^T = U_t \underbrace{V_t^T V_t}_{=G_t} U_t^T,$$

  with reduced Gramian $G_t$ (calculated recursively for all $t$).

  If $S_t$ contains $r_t$ dominant eigenvectors of $G_t \rightsquigarrow W_t = U_t S_t$.

- Remember: $\tilde{B}_t = [W_{t_2}^H \otimes W_{t_1}^H] W_t$

$$\begin{aligned}\tilde{B}_t &= [S_{t_2}^H U_{t_2}^H \otimes S_{t_1}^H U_{t_1}^H] U_t S_t \\ &= [S_{t_2}^H U_{t_2}^H \otimes S_{t_1}^H U_{t_1}^H](U_{t_2} \otimes U_{t_1}) B_t S_t = [S_{t_2}^H \otimes S_{t_1}^H] B_t S_t.\end{aligned}$$

- In `htucker`: `truncate(x,opts)`. Complexity $\mathcal{O}(dnr^2 + dr^4)$.

# Conclusions

`htucker`:

- Convenient MATLAB implementation of hierarchical Tucker format.
- Plenty of utilities and examples hopefully get you started.

  i.e., there is no documentation yet.
- Current version 0.8. (We are open to suggestions!)

Coming soon:

- Application to high-dimensional parabolic PDEs (R. Andreev)

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Thank you for your attention!