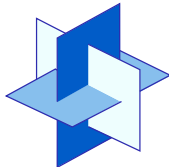
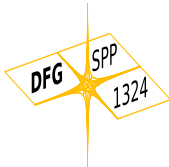


# Tensor networks, TT (Matrix Product States) and Hierarchical Tucker decomposition

R. Schneider (TUB Matheon)

John von Neumann Lecture – TU Munich, 2012



## Setting - Tensors

$V_\nu := \mathbb{R}^n$  ,  $\mathcal{H}_d = \mathcal{H} := \bigotimes_{\nu=1}^d V_\nu$   $d$ -fold tensor product Hilbert-s.,

$$\mathcal{H} \simeq \{(x_1, \dots, x_d) \mapsto U(x_1, \dots, x_d) \in \mathbb{R} : x_i = 1, \dots, n_i\} .$$

The function  $U \in \mathcal{H}$  will be called an **order  $d$ -tensor**.

For notational simplicity, we often consider  $n_i = n$ . Here  $x_1, \dots, x_d \in \{1, \dots, n\}$  will be called **variables** or **indices**.

$$\mathbf{k} \mapsto U(k_1, \dots, k_d) = (U_{k_1, \dots, k_d}) , \quad k_i = 1 \dots, n_i .$$

Or in index (vectorial) notation

$$\mathbf{U} = (U_{k_1, \dots, k_d})_{k_i=0, 1 \leq i \leq d}^{n_i}$$

$\dim \mathcal{H} = n^d$  curse of dimensions!!!

E.g. wave function  $\Psi(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N)$

# Contracted tensor representations

*Espig & Hackbusch & Handschuh & S.*

Let  $V_\nu := \mathbb{R}^{r_\nu}$

$$\mathcal{K}_K = \mathcal{K} := \bigotimes_{\nu=1}^K V_\nu \quad d\text{-fold tensor product space,}$$

$$\mathcal{K} \simeq \{(k_1, \dots, k_K) \mapsto V(k_1, \dots, k_K) : k_i = 1, \dots, r_i\}.$$

Here  $k_1, \dots, k_N$  will be called **contraction variables**,

$x_1, \dots, x_d$  will be called **exterior variables**.

We define an order  $d + K$  tensor product space

$$\tilde{\mathcal{H}} := \mathcal{H} \otimes \mathcal{K} \simeq \{(x_1, \dots, x_d, k_1, \dots, k_K) \mapsto \tilde{U}(x_1, \dots, x_d, k_1, \dots, k_K) : \\ x_i = 1, \dots, n; 1 \leq i \leq d, k_j = 1, \dots, r_j, 1 \leq j \leq K\}.$$

# Contracted tensor representations

## Definition

Subset  $\mathcal{V}^r \subseteq \mathcal{H}$ : Let  $d < d' \leq d + K$ ,

$$U \in \mathcal{V}^r \Leftrightarrow U = \sum_{k_1}^{r_1} \dots \sum_{k_K}^{r_K} \bigotimes_{\nu=1}^{d'} u_\nu(x_\nu, k_{\nu(1)}, k_{\nu(2)}, k_{\nu(3)})$$

where  $k_{\nu(i)} \in \{k_1, \dots, k_K\}$ ,  $i = 1, 2, 3$ , and

$$\begin{aligned} & u_\nu(x_\nu, k_{\nu(1)}, k_{\nu(2)}) \quad \text{if } \nu = 1, \dots, d \\ & u_\nu(k_{\nu(1)}, k_{\nu(2)}, k_{\nu(3)}) \quad \text{if } \nu = d + 1, \dots, d', \end{aligned}$$

I.e. the  $d'$  tensors  $u_\nu(\cdot, \cdot, \cdot)$  depends at most on **3** variables!  
We will write shortly  $u_\nu(x_\nu, \mathbf{k}_\nu) \in \mathbb{R}$ , keeping in mind that  $u_\nu$  depends only on at most three variables  $x_\nu, k_{\nu(1)}, k_{\nu(2)}, k_{\nu(3)}$ .

## Example

Canonical format:  $K = 1$ ,  $d' = d$ ,  $u_\nu(x_\nu, k)$ ,  $k = 1, \dots, r$ .

# Contracted tensor representations

## Definition

Subset  $\mathcal{V}^r \subseteq \mathcal{H}$ : Let  $d < d' \leq d + K$ ,

$$U \in \mathcal{V}^r \Leftrightarrow U = \sum_{k_1}^{r_1} \dots \sum_{k_K}^{r_K} \bigotimes_{\nu=1}^{d'} u_{\nu}(x_{\nu}, k_{\nu(1)}, k_{\nu(2)}, (k_{\nu(3)}))$$

the  $d'$  tensors  $u_{\nu}(\cdot, \cdot, \cdot)$  depends at most on **3** variables! (Not necessary!)

**Complexity:**

Let  $r := \max\{r_i : i = 1, \dots, K\}$  then storage requirement is

$$\#DOF's \leq \max\{d' \times n \times r^2, d' \times r^3\}.$$

# Contracted tensor representations

- ▶ Due to the multi-linear ansatz, the present extremely general format allow differentiation and local optimization methods! (See e.g. previous talk!)
- ▶ Redundancy has not been removed, in general redundancy is enlarged.
- ▶ Closedness would be violated in general.

## Tensor networks

### Definition

A minimal **tensor network** is a representation in the above format, where each contraction variable  $k_i$ ,  $i = 1, \dots, K$ , appear exactly **twice**. In this case, they can be labeled by  $i \sim (\nu, \mu)$ ,  $1 \leq \nu \leq d'$ ,  $1 \leq \mu < \nu$ . It is often assumed, that each exterior variable  $x_j$  appear at most once!

# Tensor networks

Diagram - (Graph) of a tensor network:

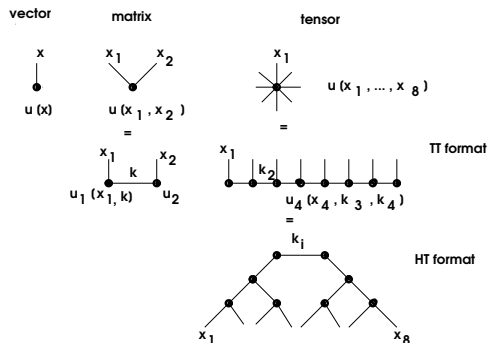


Diagramm:

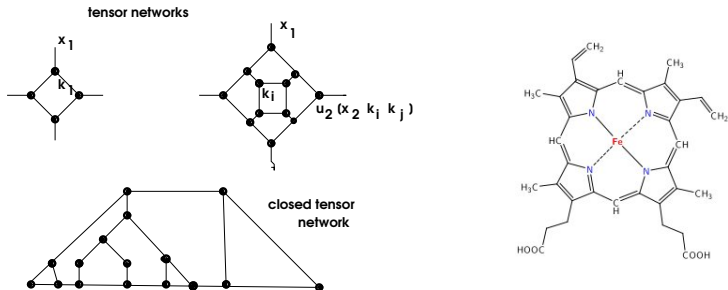
- ▶ Each **node** corresponds to a factor  $u_\nu$ ,  $\nu = 1, \dots, d'$ ,
- ▶ each **line** to a variable  $x_\nu$  or a contraction variable  $k_\mu$ .
- ▶ Since  $k_\nu$  is an edge connecting 2 tensors  $u_{\mu_1}$  and  $u_{\mu_2}$ , one has to **sum over connecting lines (edges)**.

Tensor networks has been introduced in quantum information theory.

## Example

1. TT (tensor trains, Oseledets & Tyrtysnikov ) and HT (Hackbusch & Kühn) formats are tensor networks.
2. the canonical format is not (directly) a tensor network.

### tensor networks





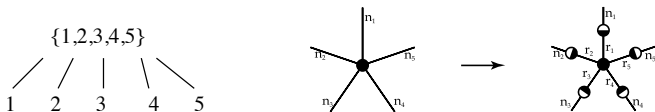
# Tensor formats

- ▶ Hierarchical Tucker format  
(HT; Hackbusch/Kühn, Grasedyck, Kressner : Tree-tensor networks)

# Tensor formats

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(HT; Hackbusch/Kühn, Grasedyck, Kressner : Tree-tensor networks)
- ▶ Tucker format (Q: MCTDH(F))

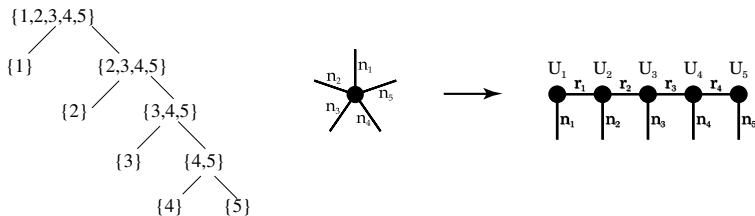
$$U(x_1, \dots, x_d) = \sum_{k_1=1}^{r_1} \dots \sum_{k_d=1}^{r_d} B(k_1, \dots, k_d) \bigotimes_{i=1}^d U_i(k_i, x_i)$$



# Tensor formats

- ▶ Hierarchical Tucker format  
(HT; Hackbusch/Kühn, Grasedyck, Kressner : Tree-tensor networks)
- ▶ Tucker format (Q: MCTDH(F))
- ▶ Tensor Train (TT-)format  
(Oseledets/Tyrtshnikov,  $\simeq$  MPS-format of quantum physics)

$$U(\underline{x}) = \sum_{k_1=1}^{r_1} \dots \sum_{k_{d-1}=1}^{r_{d-1}} \prod_{i=1}^d B_i(k_{i-1}, x_i, k_i) = \mathbf{B}_1(x_1) \cdots \mathbf{B}_d(x_d)$$



Noteable special case of HT:

TT format (Oseledets & Tyrtysnikov, 2009)

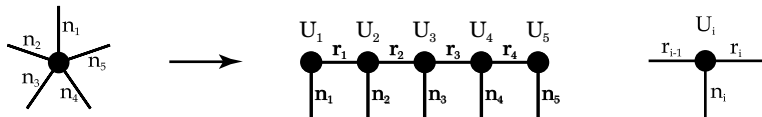
(matrix product states (MPS), Vidal 2003, Schöllwöck et al.)

TT tensor  $U$  can be written as matrix product form

$$U(\mathbf{x}) = \mathbf{U}_1(x_1) \cdots \mathbf{U}_i(x_i) \cdots \mathbf{U}_d(x_d)$$

$$= \sum_{k_1=1}^{r_1} \cdots \sum_{k_{d-1}=1}^{r_{d-1}} U_1(x_1, k_1) U_2(k_1, x_2, k_2) \cdots U_{d-1}(k_{d-2}, x_{d-1}, k_{d-1}) U_d(k_{d-1}, x_d, k_d)$$

with matrices  $\mathbf{U}_i(x_i) = (U_{k_{i-1}}^{k_i}(x_i)) \in \mathbb{R}^{r_{i-1} \times r_i}$ ,  $r_0 = r_d := 1$



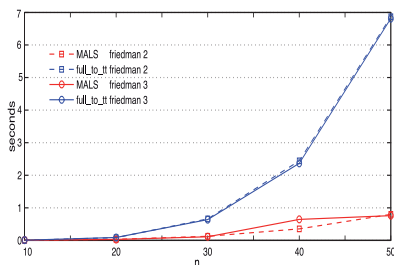
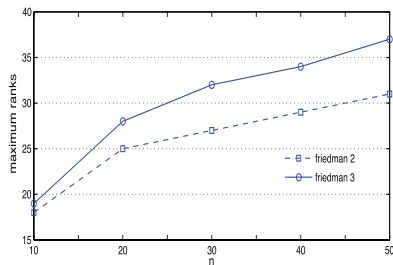
Redundancy:  $U(\mathbf{x}) = \mathbf{U}_1(x_1) \mathbf{G} \mathbf{G}^{-1} \mathbf{U}_2(x_2) \cdots \mathbf{U}_i(x_i) \cdots \mathbf{U}_d(x_d)$ .

# TT approximations of Friedman data sets

$$f_2(x_1, x_2, x_3, x_4) = \sqrt{\left(x_1^2 + \left(x_2 x_3 - \frac{1}{x_2 x_4}\right)^2\right)}$$

$$f_3(x_1, x_2, x_3, x_4) = \tan^{-1}\left(\frac{x_2 x_3 - (x_2 x_4)^{-1}}{x_1}\right)$$

on 4 –  $D$  grid,  $n$  points per dim.  $\rightsquigarrow n^4$  tensor,  $n \in \{3, \dots, 50\}$ .

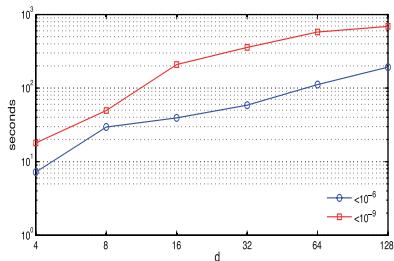
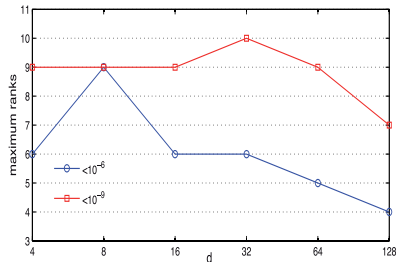


full\_to\_tt  
and MALS (with  $A = I$ )

(Oseledets, successive SVDs)  
(Holtz & Rohwedder & S.)

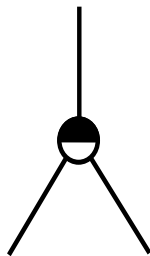
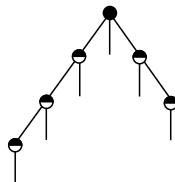
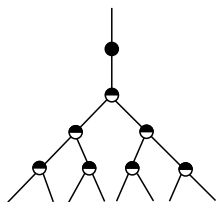
# Solution of $-\Delta U = b$

- ▶ Dimension  $d = 4, \dots, 128$  varying
- ▶ Gridsize  $n = 10$
- ▶ Right-hand-side  $b$  of rank 1
- ▶ Solution  $U$  has rank 13



# Hierarchical Tucker as subspace approximation

- 1)  $D = \{1, \dots, d\}$ , tensor space  $\mathbf{V} = \bigotimes_{j \in D} V_j$
- 2)  $T_D$  dimension partition tree, vertices  $\alpha \in T_D$  are subsets  $\alpha \subset T_D$ , root:  $\alpha = D$
- 3)  $\mathbf{V}_\alpha = \bigotimes_{j \in \alpha} V_j$  for  $\alpha \in T_D$



- 4)  $\mathbf{U}_\alpha \subset \mathbf{V}_\alpha$  subspaces of dimension  $r_\alpha$  with the characteristic nesting

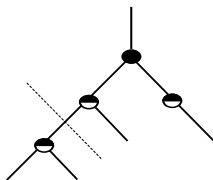
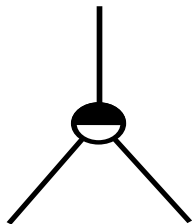
$$\mathbf{U}_\alpha \subset \mathbf{U}_{\alpha_1} \otimes \mathbf{U}_{\alpha_2} \quad (\alpha_1, \alpha_2 \text{ sons of } \alpha)$$

- 5)  $\mathbf{v} \in \mathbf{U}_D$  (w.l.o.g.  $\mathbf{U}_D = \text{span}(\mathbf{v})$ ).

# Subspace approximation: formulation with bases

$$\mathbf{U}_\alpha = \text{span} \{ \mathbf{b}_i^{(\alpha)} : 1 \leq i \leq r_\alpha \}$$

$$\mathbf{b}_\ell^{(\alpha)} = \sum_{i=1}^{r_{\alpha_1}} \sum_{j=1}^{r_{\alpha_2}} c_{ij}^{(\alpha, \ell)} \mathbf{b}_i^{(\alpha_1)} \otimes \mathbf{b}_j^{(\alpha_2)} \quad (\alpha_1, \alpha_2 \text{ sons of } \alpha \in T_D).$$



Coefficients  $c_{ij}^{(\alpha, \ell)}$  form the matrices  $C^{(\alpha, \ell)}$ .

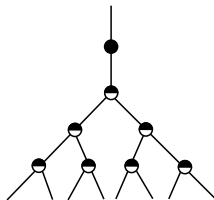
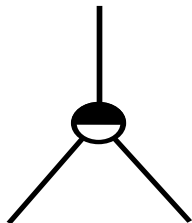
Final representation of  $\mathbf{v}$  is

$$\mathbf{v} = \sum_{i=1}^{r_D} c_i^{(D)} \mathbf{b}_i^{(D)}, \quad (\text{usually with } r_D = 1).$$



# Orthonormal basis and recursive description

We can choose  $\{\mathbf{b}_i^{(\alpha)} : 1 \leq i \leq r_\alpha\}$  orthonormal basis for  $\alpha \in T_D$ .



This is equivalent to

- 1) At the leaves ( $\alpha = \{j\}, j \in D$ ):  $\{\mathbf{b}_i^{(j)} : 1 \leq i \leq r_j\}$  is chosen orthonormal
- 2) The matrices  $\{\mathbf{C}^{(\alpha, \ell)} : 1 \leq \ell \leq r_\alpha\}$  are orthonormal (w.r.t. the Frobenius scalar product).

# Hierarchical Tucker tensors

- ▷ Canonical decomposition
- ▷ Subspace approach (Hackbusch/Kühn, 2009)

(Example:  $d = 5$ ,  $\mathbf{U}_i \in \mathbb{R}^{n \times k_i}$ ,  $\mathbf{B}_t \in \mathbb{R}^{k_t \times k_{t_1} \times k_{t_2}}$ )

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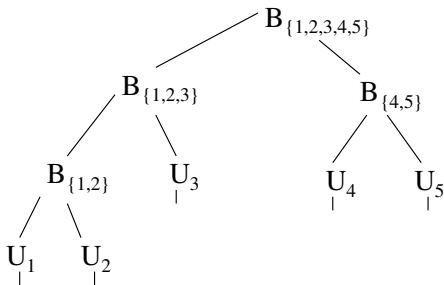
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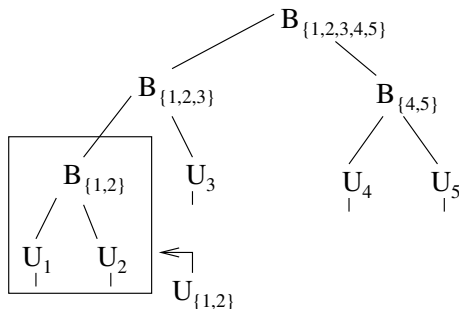
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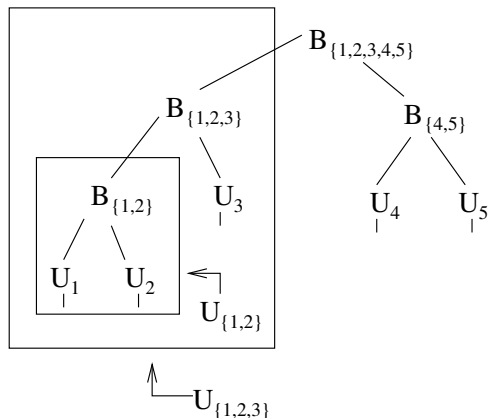
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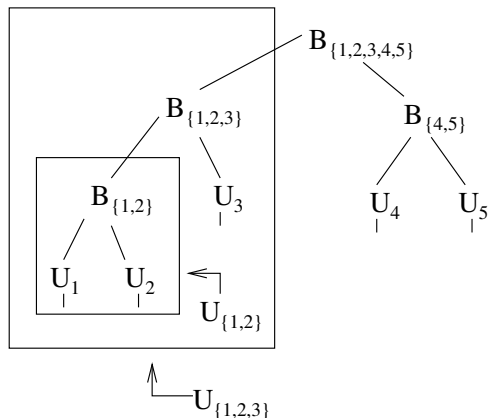
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# HOSVD bases (Hackbusch)

1) Assume  $r_D = 1$ . Then

$$\mathbf{C}^{(D,1)} = \Sigma_\alpha := \text{diag}\{\sigma_1^{(D)}, \dots\},$$

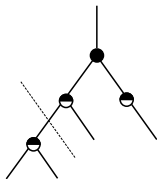
where  $\sigma_i^{(D)}$  are the singular values of  $\mathcal{M}_{\alpha_1}(\mathbf{v})$

2) For non-leaf vertices  $\alpha \in T_D$ ,  $\alpha \neq D$ , we have

$$\sum_{\ell=1}^{r_\alpha} (\sigma_\ell^{(\alpha)})^2 \mathbf{C}^{(\alpha,\ell)} \mathbf{C}^{(\alpha,\ell)\mathbf{H}} = \Sigma_{\alpha_1}^2,$$

$$\sum_{\ell=1}^{r_\alpha} (\sigma_\ell^{(\alpha)})^2 \mathbf{C}^{(\alpha,\ell)\mathbf{T}} \overline{\mathbf{C}^{(\alpha,\ell)}} = \Sigma_{\alpha_2}^2,$$

where  $\alpha_1, \alpha_2$  are the first and second son of  $\alpha \in T_D$  and  $\Sigma_{\alpha_i}$  the diagonal of the singular values of  $\mathcal{M}_{\alpha_i}(\mathbf{v})$ .



## Historical remarks – hierarchical Tucker approx.

Physics: (I do not have suff. complete knowledge)

The ideas are well established in many body quantum physics, quantum optics and quantum information theory

1. DMRG: S. White (91)
2. MPS: Roemmer & Ostlund (94), Vidal (03), Verstraete et al.
3. (tree) tensor networks : Verstrate, Cirac, Schollwöck, Wolf, Eisert .... (?)
4. MERA, PEPS, .....
5. Chemistry: Multilevel MCTDH  $\simeq$  HT : Meyer et al. (2000)

Mathematics: Completely new in tensor product approximation

1. Khoromskij et al. (2006), remark about multi level Tucker
2. Lubich (book) (2008): review about Meyers paper
3. HT - Hackbusch (2009) et al.: Introduction of the subspace approximation!!!!
4. Grasedyck (2009): HT -sequential SVD
5. Oseledets & Tyrtishnikov (2009): TT and sequential SVD

# Successive SVD for e.g. TT tensors

- Vidal (2003), Oseledets (2009), Grasedyck (2009)

## 1. Matricisation - unfolding

$$F(x_1, \dots, x_d) \approx \mathbf{F}_{x_1}^{x_2, \dots, x_d} .$$

low rank approximation up to an error  $\epsilon_1$ , e.g. by SVD.

$$\mathbf{F}_{x_1}^{x_2, \dots, x_d} = \sum_{k_1=0}^{r_1} \mathbf{u}_{x_1}^{k_1} \mathbf{v}_{k_1}^{x_2, \dots, x_d} ,$$

$$U_1(x_1, k_1) := \mathbf{u}_{x_1}^{k_1} , \quad k_1 = 1, \dots, r_1 .$$

## 2. Decompose $V(k_1, x_2, \dots, x_d)$ via matricisation up to an accuracy $\epsilon_2$ ,

$$\mathbf{v}_{k_1, x_2}^{x_3, \dots, x_d} = \sum_{k_2}^{r_2} \mathbf{u}_{k_1, x_2}^{k_2} \mathbf{v}_{k_2}^{x_3, \dots, x_d}$$

$$U_2(k_1, x_2, k_2) := \mathbf{u}_{k_1, x_2}^{k_2} .$$

## 3. repeat with $V(k_2, x_3, \dots, x_d)$ until one ends with $[\mathbf{v}_{k_{d-1}, x_d}] \mapsto U_d(k_{d-1}, x_d)$ .

## Example

The function

$$U(x_1, \dots, x_d) = x_1 + \dots + x_d \in \mathcal{H}$$

in canonical representation

$$U(x_1, \dots, x_d) = x_1 \cdot 1 \dots 1 + 1 \cdot x_2 \cdot 1 \dots 1 + \dots + 1 \dots 1 \cdot x_d$$

In Tucker format, let

$\mathbf{U}_{i,1} = \mathbf{1}$ ,  $\mathbf{U}_{i,2} = x_i$  be the basis of  $\mathbf{U}_i$  (non-orthogonal),  $r_i = 2$ .

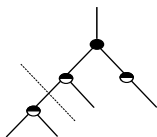
$U$  in TT or MPS representation

$$U(\underline{x}) = x_1 + \dots + x_d = (x_1 \quad 1) \begin{pmatrix} 1 & 0 \\ x_2 & 1 \end{pmatrix} \cdot \dots \cdot \begin{pmatrix} 1 & 0 \\ x_{d-1} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x_d \end{pmatrix}.$$

(non-orthogonal),  $r_1 = \dots = r_{d-1} = 2$

## Successive SVD for e.g. TT tensors

The above algorithm can be extended to HT tensors!



### Error analysis

- ▶ Quasi best approximation

$$\begin{aligned}\|F(\mathbf{x}) - \mathbf{U}(x_1) \dots \mathbf{U}_d(x_d)\|_2 &\leq \left(\sum_{i=1}^{d-1} \epsilon_i^2\right)^{1/2} \\ &\leq \sqrt{d-1} \inf_{U \in \mathcal{T}^{\leq r}} \|F(\mathbf{x}) - U(\mathbf{x})\|_2.\end{aligned}$$

- ▶ Exact recovery: if  $U \in \mathcal{T}^{\leq r}$ , then it will be recovered exactly!  
(up to rounding errors)

## Ranks of TT and HT tensors

The minimal numbers  $r_i$  for a TT or HT representation of a tensor  $U$  is well defined.

1. The optimal ranks  $r_i$ ,  $\underline{r} = (r_1, \dots, r_{d-1})$ , of the TT decomposition are equal to the ranks of the following matrices,  $i = 1, \dots, d-1$

$$r_i = \text{rank of } \mathbf{A}_i = U_{x_1, \dots, x_i}^{x_{i+1}, \dots, x_d}.$$

2. If  $\nu \subset D$  then  $\mu := D \setminus \nu$  the the *mode*  $\nu$ -rank  $r_\nu$  is given by

$$r_\nu = \text{rank of } \mathbf{A}_i = U_{\underline{x}_\nu}^{\underline{x}_\mu}.$$

(If  $\nu = \{1, 2, 7, 8\}$  and  $\mu = \{3, 4, 5, 6\}$  then  $\underline{x}_\nu = (x_1, x_2, x_7, x_8)$ .)

# Closedness

A tree  $T_D$  is characterized by the property, if one remove one edge yields two separate trees.

Observation: Let  $\mathbf{A}_i$  with ranks  $\text{rank}\mathbf{A}_i \leq r$ . If

$\lim_{i \rightarrow \infty} \|\mathbf{A}_i - \mathbf{A}\|_2 = 0$  then  $\text{rank}\mathbf{A} \leq r: \Rightarrow$  closedness of Tucker and HT tensor in  $\mathbb{T}^{\leq r}$  (Falco & Hackbusch).

$$\boxed{\mathbb{T}^{\leq r} = \bigcup_{s \leq r} \mathbb{T}_s \subset \mathcal{H} \text{ is closed!}} \quad \text{due to Hackbusch \& Falco}$$

Landsberg & Ye: If a tensor network has not a tree structure, the set of all tensor of this form need not to be closed!

## Landsbergs result - tensor networks

Let  $\mu$  are the vertices and  $s_\mu \in S_\mu$  are incident edges of a vertex  $\mu$ , and  $V_\mu$  the vector space attached to it. (it can be empty!)

A vertex  $\mu$  is called *super critical* if

$$\dim V_\mu \geq \prod_{s(\mu) \in S(\mu)} r_{s(\mu)},$$

and *critical* if  $\dim V_\mu = \prod_{s(\mu) \in S(\mu)} r_{s(\mu)}$

### Lemma

*Any supercritical vertex can be reduced to a critical one by Tucker decomposition.*

### Theorem (Landsberg-Ye)

*If a (proper) loop a tensor network contains only (super)-critical vertices, then the network is **not (Zariski)-closed**.*

i.e. if the ranks are too small! For  $\bigotimes_{i=1}^d \mathbb{C}^2$ , i.e.  $n = 2$ , Landsbergs result has no consequences.



## Summary

For Tucker and HT redundancy can be removed (see next talk)

Table: Comparison

	canonical	Tucker	HT
complexity	$\mathcal{O}(ndr)$ ++	$\mathcal{O}(r^d + ndr)$ -	$\mathcal{O}(ndr + dr^3)$ TT- $\mathcal{O}(ndr^2)$ +
rank	no $r_c \geq$	defined $r_T$	defined $r_{HT}, r_T \leq r_{HT}$
closedness	no	yes	yes
essential redundancy	yes	no	no
recovery	??	yes	yes
quasi best approx.	no	yes	yes
best approx.	no	exist but NP hard	exist but NP hard

# Thank you for your attention.

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