

Numerical Tensor Calculus

Wolfgang Hackbusch Wolfgang Hackbusch

Max-Planck-Institut für *Mathematik in den Naturwissenschaften*
and University of Kiel



Inselstr. 22-26, D-04103 Leipzig, Germany
wh@mis.mpg.de

http://www.mis.mpg.de/scicomp/hackbusch_e.html

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Tensorisation

1 Introduction: Tensors

1.1 Where do large-scale tensors appear?

The tensor space $\mathbf{V} = V_1 \otimes V_2 \otimes \dots \otimes V_d$ with vector spaces V_j ($1 \leq j \leq d$) is defined as (closure of)

$$\text{span}\{v^{(1)} \otimes v^{(2)} \otimes \dots \otimes v^{(d)} : v^{(j)} \in V_j\}.$$

Finite dimensional case:

$$V_j = \mathbb{R}^{n_j} = \mathbb{R}^{I_j} \text{ with } I_j = \{1, \dots, n_j\}.$$

Set $\mathbf{I} := I_1 \times I_2 \times \dots \times I_d$, then $\mathbf{V} \simeq \mathbb{R}^{\mathbf{I}}$, i.e., $\mathbf{v} = (v_{\mathbf{i}})_{\mathbf{i} \in \mathbf{I}}$.

Tensor product: $\mathbf{v} = v^{(1)} \otimes v^{(2)} \otimes \dots \otimes v^{(d)} \in \mathbb{R}^{\mathbf{I}}$ with $v^{(j)} \in \mathbb{R}^{I_j}$ defined as

$$v_{\mathbf{i}} = v_{i_1, \dots, i_d} = v[i_1, \dots, i_d] = v_{i_1}^{(1)} \cdot v_{i_2}^{(2)} \cdot \dots \cdot v_{i_d}^{(d)} \quad \text{for } \mathbf{i} = (i_1, \dots, i_d) \in \mathbf{I}.$$

1.1.1 Functions

Multivariate functions f defined on a Cartesian product

$$\Omega = \Omega_1 \times \Omega_2 \times \dots \times \Omega_d$$

are tensors.

For instance,

$$L^2(\Omega) = L^2(\Omega_1) \otimes L^2(\Omega_2) \otimes \dots \otimes L^2(\Omega_d).$$

Tensor product of univariate functions:

$$\left(\bigotimes_{j=1}^d f_j \right) (x_1, x_2, \dots, x_d) := \prod_{j=1}^d f_j(x_j).$$

The multivariate function may be the solution of a partial differential equation.

The numerical treatment replaces functions by finite-dimensional analogues
(\rightarrow grid functions, finite-element functions).

1.1.2 Grid Functions

Discretisation in *product grids* $\omega = \omega_1 \times \omega_2 \times \dots \times \omega_d$,
e.g., ω_j regular grid with n_j grid points.

Total number of grid points $N = \prod_{j=1}^d n_j$, e.g., n^d . Tensor space:

$$\mathbb{R}^N \simeq \mathbb{R}^{n_1} \otimes \mathbb{R}^{n_2} \otimes \dots \otimes \mathbb{R}^{n_d}.$$

Small discretisation errors require large dimensions n_j .

Challenge: Huge dimensions like in ...

1) $n = 1\,000\,000$ and $d = 3$

2) $n = 1000$ and $d = 1000 \Rightarrow$

$$N = 1000^{1000} = 10^{3000}.$$

1.1.3 Matrices or Operators

Let $\mathbf{V} = V_1 \otimes V_2 \otimes \dots \otimes V_d$, $\mathbf{W} = W_1 \otimes W_2 \otimes \dots \otimes W_d$ be tensor spaces,

$A_j : V_j \rightarrow W_j$ linear mappings ($1 \leq j \leq d$).

The tensor product (*Kronecker product*)

$$\mathbf{A} = A_1 \otimes A_2 \otimes \dots \otimes A_d : \mathbf{V} \rightarrow \mathbf{W}$$

is the mapping

$$\mathbf{A} : v^{(1)} \otimes v^{(2)} \otimes \dots \otimes v^{(d)} \mapsto A_1 v^{(1)} \otimes A_2 v^{(2)} \otimes \dots \otimes A_d v^{(d)}.$$

If $A_j \in \mathbb{R}^{n \times n}$ then $\mathbf{A} \in \mathbb{R}^{n^d \times n^d}$.

Example: Poisson problem $-\Delta u = f$ in $[0, 1]^d$, $u = 0$ on Γ .

The differential operator has the form

$$L = \frac{\partial^2}{\partial x_1^2} \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes \frac{\partial^2}{\partial x_d^2}.$$

Discretise by difference scheme with n grid points per direction.

The system matrix is

$$\mathbf{A} = T_1 \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes T_d.$$

Challenge: Approximate the inverse of $\mathbf{A} \in \mathbb{R}^{N \times N}$,

where $n = d = 1000$, so that

$$N = n^d = 1000^{1000} = 10^{3000}.$$

Later result: required storage: $O(dn \log^2 \frac{1}{\varepsilon})$

1.2 Tensor Operations

addition: $\mathbf{v} + \mathbf{w}$,

scalar product: $\langle \mathbf{v}, \mathbf{w} \rangle$

matrix-vector multiplication: $\left(\bigotimes_{j=1}^d A^{(j)} \right) \left(\bigotimes_{j=1}^d v^{(j)} \right) = \bigotimes_{j=1}^d A^{(j)} v^{(j)}$,

Hadamard product: $(\mathbf{v} \odot \mathbf{w})[\mathbf{i}] = \mathbf{v}[\mathbf{i}] \mathbf{w}[\mathbf{i}]$, pointwise product of functions

$$\left(\bigotimes_{j=1}^d v^{(j)} \right) \odot \left(\bigotimes_{j=1}^d w^{(j)} \right) = \bigotimes_{j=1}^d v^{(j)} \odot w^{(j)},$$

convolution: $\mathbf{v}, \mathbf{w} \in \bigotimes_{j=1}^d \mathbb{R}^n : \mathbf{u} = \mathbf{v} \star \mathbf{w}$ with $u_{\mathbf{i}} = \sum_{0 \leq \mathbf{k} \leq \mathbf{i}} v_{\mathbf{i}-\mathbf{k}} w_{\mathbf{k}}$

$$\left(\bigotimes_{j=1}^d v^{(j)} \right) \star \left(\bigotimes_{j=1}^d w^{(j)} \right) = \bigotimes_{j=1}^d v^{(j)} \star w^{(j)}.$$

1.3 High-Dimensional Problems in Practice

- 1) boundary value problems $Lu = f$ in cubes or $\mathbb{R}^3 \Rightarrow d = 3, n_j$ large
- 2) Hartree-Fock equations (as 1))
- 3) Schrödinger equation ($d = 3 \times$ number of electrons + antisymmetry)
- 4) bvp $L(p)u = f$ with parameters $p = (p_1, \dots, p_m) \Rightarrow d = m + 1$
- 5) bvp with stochastic coefficients \Rightarrow as 4) with $m = \infty$
- 6) coding of a d -variate function in Cartesian product $\Rightarrow d = d$
- 7) ...
- 8) Lyapunov equation $(A \otimes I + I \otimes A) \mathbf{x} = \mathbf{b}$

2 Tensor Representations

How to represent tensors with n^d entries by few data?

Classical formats:

- r -Term Format (Canonical Format)
- Tensor Subspace Format (Tucker Format)

More recent:

- Hierarchical Tensor Format

2.1 r -Term Format (Canonical Format)

By definition, any algebraic tensor $\mathbf{v} \in \mathbf{V} = V_1 \otimes V_2 \otimes \dots \otimes V_d$ has a representation

$$\mathbf{v} = \sum_{\rho=1}^r v_{\rho}^{(1)} \otimes v_{\rho}^{(2)} \otimes \dots \otimes v_{\rho}^{(d)} \quad \text{with } v_{\rho}^{(j)} \in V_j$$

and suitable r . Set

$$\mathcal{R}_r := \left\{ \sum_{\rho=1}^r v_{\rho}^{(1)} \otimes v_{\rho}^{(2)} \otimes \dots \otimes v_{\rho}^{(d)} : v_{\rho}^{(j)} \in V_j \right\}$$

Storage: rdn (for $n = \max \dim V_j$).

If r is of moderate size, this format is advantageous.

Often, a tensor \mathbf{v} is replaced by an approximation $\mathbf{v}_{\varepsilon} \in \mathcal{R}_r$ with $r = r(\varepsilon)$.

$$\text{rank}(\mathbf{v}) := \min\{r : \mathbf{v} \in \mathcal{R}_r\}, \quad \mathcal{R}_r := \{\mathbf{v} \in \mathbf{V} : \text{rank}(\mathbf{v}) \leq r\}.$$

Recall the matrix \mathbf{A} discretising the Laplace equation:

$$\mathbf{A} = T_1 \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes T_d.$$

REMARK: $\mathbf{A} \in \mathcal{R}_d$ and $\text{rank}(\mathbf{A}) = d$ (tensor rank, not matrix rank).

T_j : tridiagonal matrices of size $n \times n$.

Size of \mathbf{A} : $N \times N$ with $N = n^d$.

E.g., $n = d = 1000 \implies N = n^d = 1000^{1000} = 10^{3000}$.

We aim at the **inverse** of $\mathbf{A} \in \mathbb{R}^{N \times N}$.

Solution: $\mathbf{A}^{-1} \approx \mathbf{B}_r$ with \mathbf{B}_r of the form

$$\mathbf{B}_r = \sum_{i=1}^r a_i \bigotimes_{j=1}^d \exp(-b_i T_j),$$

where $a_i, b_i > 0$ are explicitly known.

Proof. Approximate $1/x$ in $[1, \infty)$ by exponential sums $E_r(x) = \sum_{i=1}^r a_i \exp(-b_i x)$. The best approximation satisfies

$$\left\| \frac{1}{\bullet} - E_r(\cdot) \right\|_{\infty, [1, \infty)} \leq O(\exp(-cr^{1/2})).$$

For a positive definite matrix with $\sigma(\mathbf{A}) \subset [1, \infty)$, $E_r(\mathbf{A})$ approximates \mathbf{A}^{-1} with

$$\left\| E_r(\mathbf{A}) - \mathbf{A}^{-1} \right\|_2 \leq O(\exp(-cr^{1/2})).$$

In the case of $\mathbf{A} = T_1 \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes T_d$ one obtains

$$\mathbf{B}_r := E_r(\mathbf{A}) = \sum_{i=1}^r a_i \bigotimes_{j=1}^d \exp(-b_i T_j) \in \mathcal{R}_r.$$

Representation versus Decomposition

$P := (\times_{j=1}^d V_j)^r$ parameter set.

Representation of a tensor:

$$\varphi : P \longrightarrow \mathcal{R}_r \subset \mathbf{V}.$$

Injectivity of φ not required, $\text{rank}(\varphi(p)) \leq r$.

Let $\text{rank}(\mathbf{v}) = r$. Under certain conditions the representation of $\mathbf{v} = \varphi(p)$ is *essentially* unique. This allows the **decomposition**

$$\varphi^{-1} : \mathcal{R}_r \longrightarrow P.$$

Operations with Tensors and Truncations

$$\mathbf{A} = \sum_{\nu=1}^r \bigotimes_{j=1}^d A_{\nu}^{(j)} \in \mathcal{R}_r, \quad \mathbf{v} = \sum_{\nu=1}^s \bigotimes_{j=1}^d v_{\nu}^{(j)} \in \mathcal{R}_s$$

\Rightarrow

$$\mathbf{w} := \mathbf{A}\mathbf{v} = \sum_{\nu=1}^r \sum_{\mu=1}^s \bigotimes_{j=1}^d A_{\nu}^{(j)} v_{\mu}^{(j)} \in \mathcal{R}_{rs}$$

Because of the increased representation rank rs , one must apply a **truncation** $\mathbf{w} \mapsto \mathbf{w}' \in \mathcal{R}_{r'}$ with $r' < rs$.

Unfortunately, truncation to lower rank is not straightforward in the r -term format.

There are also other disadvantages of the r -term format

Numerical Difficulties because of Non-Closedness

In general, \mathcal{R}_r is *not closed*. Example: a, b linearly independent and

$$\begin{aligned} \mathbf{v} &= a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a \in \mathcal{R}_3 \setminus \mathcal{R}_2 \\ \mathbf{v} &= \underbrace{(b + na) \otimes \left(a + \frac{1}{n}b\right) \otimes a + a \otimes a \otimes (b - na)}_{\mathbf{v}_n \in \mathcal{R}_2} - \frac{1}{n}b \otimes b \otimes a. \end{aligned}$$

Here, the terms of \mathbf{v}_n grow like $O(n)$, while the result is of size $O(1)$. This implies *numerical cancellation*: $\log_2 n$ binary digits of \mathbf{v}_n are lost. We say that the sequence $\{\mathbf{v}_n\}$ is unstable.

Proposition: Suppose $\dim(V_j) < \infty$ and $\mathbf{v} \in \mathbf{V} = \bigotimes_{j=1}^d V_j$.

A stable sequence $\mathbf{v}_n \in \mathcal{R}_r$ with $\lim \mathbf{v}_n = \mathbf{v}$ exists if and only if $\mathbf{v} \in \mathcal{R}_r$.

Conclusion: If $\mathbf{v} = \lim \mathbf{v}_n \notin \mathcal{R}_r$, the sequence $\mathbf{v}_n \in \mathcal{R}_r$ is unstable.

Best approximation problem: Let $\mathbf{v}^* \in \mathbf{V}$. Try to find $\mathbf{v} \in \mathcal{R}_r$ with

$$\|\mathbf{v}^* - \mathbf{v}\| = \inf\{\|\mathbf{v}^* - \mathbf{w}\| : \mathbf{w} \in \mathcal{R}_r\}.$$

This optimisation problem need **not be solvable**.

De Silva–Lim (2008): Tensors without a best approximation have a positive measure ($\mathbb{K} = \mathbb{R}$).

2.2 Tensor Subspace Format (Tucker Format)

2.2.1 Definition of $\mathcal{T}_{\mathbf{r}}$

Implementational description: $\mathcal{T}_{\mathbf{r}}$ with $\mathbf{r} = (r_1, \dots, r_d)$ contains all tensors of the form

$$\mathbf{v} = \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathbf{a}[i_1, \dots, i_d] \bigotimes_{j=1}^d b_{i_j}^{(j)}$$

with some vectors $\{b_{i_j}^{(j)} : 1 \leq i_j \leq r_j\} \subset V_j$ possibly with $r_j \ll n_j$ and $\mathbf{a}[i_1, \dots, i_d] \in \mathbb{R}$.

The **core tensor** \mathbf{a} has $\prod_{j=1}^d r_j$ entries.

Algebraic description:

Tensor space $\mathbf{V} = V_1 \otimes V_2 \otimes \dots \otimes V_d$. Choose subspaces $U_j \subset V_j$ and consider

the **tensor subspace** $\mathbf{U} = \bigotimes_{j=1}^d U_j$. Then

$$\mathcal{T}_{\mathbf{r}} := \bigcup_{\dim(U_j) \leq r_j} \bigotimes_{j=1}^d U_j.$$

Short Notation

$$\mathbf{v} = \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathbf{a}[i_1, \dots, i_d] \bigotimes_{j=1}^d b_{i_j}^{(j)}.$$

Define matrices $B^{(j)} := [b_1^{(j)} \cdots b_{r_j}^{(j)}]$ and $\mathbf{B} := \bigotimes_{j=1}^d B^{(j)}$.

Then

$$\mathbf{v} = \mathbf{B}\mathbf{a}$$

2.2.2 Matricisation and Tucker Ranks

Let $\mathbf{V} = \mathbb{R}^{n_1} \otimes \mathbb{R}^{n_2} \otimes \dots \otimes \mathbb{R}^{n_d}$, fix $j \in \{1, \dots, d\}$, set $n_{[j]} := \prod_{k \neq j} n_k$.

The j -th *matricisation* maps a **tensor** $\mathbf{v} \in \mathbf{V}$ into a **matrix**

$$M_j \in \mathbb{R}^{n_j \times n_{[j]}}$$

defined by

$$M_j[i_j, \mathbf{i}_{[j]}] := \mathbf{v}[i_1, \dots, i_d] \quad \text{for } \mathbf{i}_{[j]} := (i_1, \dots, i_{j-1}, i_{j+1}, \dots, i_d).$$

The isomorphism $\mathcal{M}_j : \mathbf{V} \rightarrow \mathbb{R}^{n_j \times n_{[j]}}$ is called the j -th *matricisation*.

Tucker rank or j -th rank:

$$r_j = \text{rank}_j(\mathbf{v}) := \text{rank}(\mathcal{M}_j(\mathbf{v})) \quad \text{for } 1 \leq j \leq d.$$

Sometimes, $\mathbf{r} := (r_1, \dots, r_d)$ is called the *multilinear rank* of \mathbf{v} .

Example: $\mathbf{v} \in \mathbf{V} := \mathbb{R}^2 \otimes \mathbb{R}^2 \otimes \mathbb{R}^2 \otimes \mathbb{R}^2$. Then $\mathcal{M}_2(\mathbf{v})$ belongs to $\mathbb{R}^{2 \times 8}$:

$$\mathcal{M}_2(\mathbf{v}) = \begin{pmatrix} \mathbf{v}_{1111} & \mathbf{v}_{1112} & \mathbf{v}_{1121} & \mathbf{v}_{1122} & \mathbf{v}_{2111} & \mathbf{v}_{2112} & \mathbf{v}_{2121} & \mathbf{v}_{2122} \\ \mathbf{v}_{1211} & \mathbf{v}_{1212} & \mathbf{v}_{1221} & \mathbf{v}_{1222} & \mathbf{v}_{2211} & \mathbf{v}_{2212} & \mathbf{v}_{2221} & \mathbf{v}_{2222} \end{pmatrix}.$$

2.2.3 Important Properties

Alternative definition of \mathcal{T}_r :

$$\mathcal{T}_r = \left\{ \mathbf{v} \in \mathbf{V} : \text{rank}_j(\mathbf{v}) \leq r_j \text{ for all } 1 \leq j \leq d \right\}.$$

Later we shall prove:

- Also for $\dim V_j = \infty$, $\text{rank}_j(\mathbf{v})$ can be defined.
- \mathcal{T}_r is weakly closed.
- If \mathbf{V} is a reflexive Banach space, the best approximation problem

$$\inf_{\mathbf{u} \in \mathcal{T}_r} \|\mathbf{v} - \mathbf{u}\| = \|\mathbf{v} - \mathbf{u}_{\text{best}}\|$$

has a solution $\mathbf{u}_{\text{best}} \in \mathcal{T}_r$.

Choice of Vectors $b_i^{(j)}$

Let $\mathbf{v} \in \bigotimes_{j=1}^d U_j$. Representation of U_j by

1) generating system $\{b_i^{(j)}\}$ with $U_j = \text{span}_i b_i^{(j)}$,

2) basis $\{b_i^{(j)}\}_{i=1}^{r_j}$ ($r_j = \dim U_j$)

3) orthonormal basis (good numerical properties!)

4) special orthonormal basis: HOSVD basis

2.2.4 HOSVD: Higher Order Singular Value Decomposition

Diagonalisation:

$$\mathbb{R}^{n_j \times n_j} \ni \mathcal{M}_j(\mathbf{v})\mathcal{M}_j(\mathbf{v})^\top = \sum_{i=1}^{\text{rank}_j(\mathbf{v})} (\sigma_i^{(j)})^2 b_i^{(j)}(b_i^{(j)})^\text{H}.$$

$\sigma_i^{(j)}$: j -th singular values; $\{b_i^{(j)} : 1 \leq i \leq \text{rank}_j(\mathbf{v})\}$: *HOSVD basis* (orthonormal!).

Truncation: Let $\mathbf{v} = \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} \mathbf{a}[i_1, \dots, i_d] \bigotimes_{j=1}^d b_{i_j}^{(j)} \in \mathcal{T}_{\mathbf{r}}$ with HOSVD basis vectors $b_i^{(j)}$. For $\mathbf{s} = (s_1, \dots, s_d) \leq \mathbf{r}$ set

$$\mathbf{u}_{\text{HOSVD}} = \sum_{i_1=1}^{s_1} \cdots \sum_{i_d=1}^{s_d} \mathbf{a}[i_1, \dots, i_d] \bigotimes_{j=1}^d b_{i_j}^{(j)} \in \mathcal{T}_{\mathbf{s}}.$$

Quasi-optimality:

$$\|\mathbf{v} - \mathbf{u}_{\text{HOSVD}}\| \leq \left(\sum_{j=1}^d \sum_{i=s_j+1}^{r_j} (\sigma_i^{(j)})^2 \right)^{1/2} \leq d^{1/2} \|\mathbf{v} - \mathbf{u}_{\text{best}}\| \quad (\mathbf{u}_{\text{best}} \in \mathcal{T}_{\mathbf{s}}).$$

Conclusion concerning the traditional formats:

1. r -term format \mathcal{R}_r

- advantage: low storage cost rdn
- disadvantage: difficult truncation, numerical instability may occur

2. tensor subspace format \mathcal{T}_r

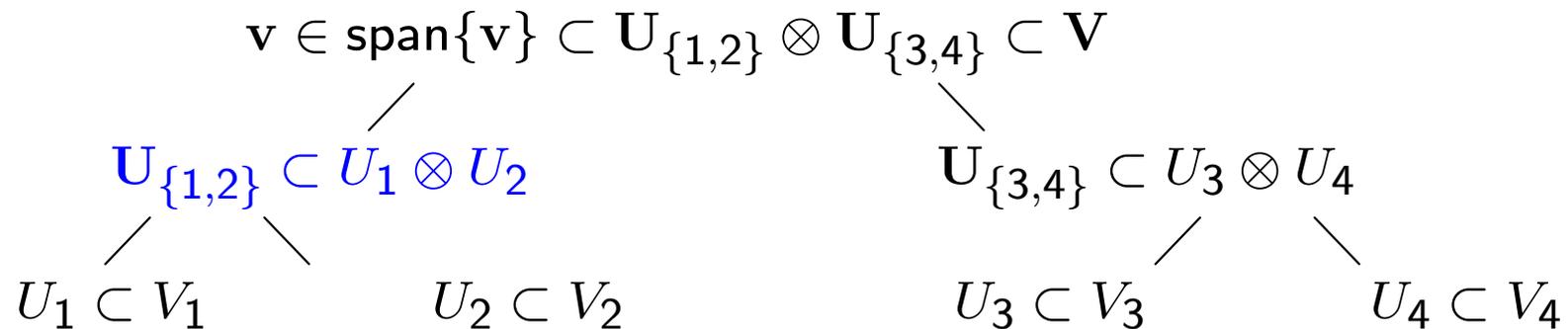
- advantage: stable and quasi-optimal truncation
- disadvantage: exponentially expensive storage for core tensor \mathbf{a}

The next format combines the advantages.

3 Hierarchical Format

3.1 Dimension Partition Tree

Example: $\mathbf{v} \in \mathbf{V} = V_1 \otimes V_2 \otimes V_3 \otimes V_4$. There are subspaces such that



Optimal subspaces are $\mathbf{U}_\alpha := U_\alpha^{\min}(\mathbf{v})$.

Dimension partition tree:

Any binary tree with root $D := \{1, \dots, d\}$ and leaves $\{1\}, \{2\}, \dots, \{d\}$.

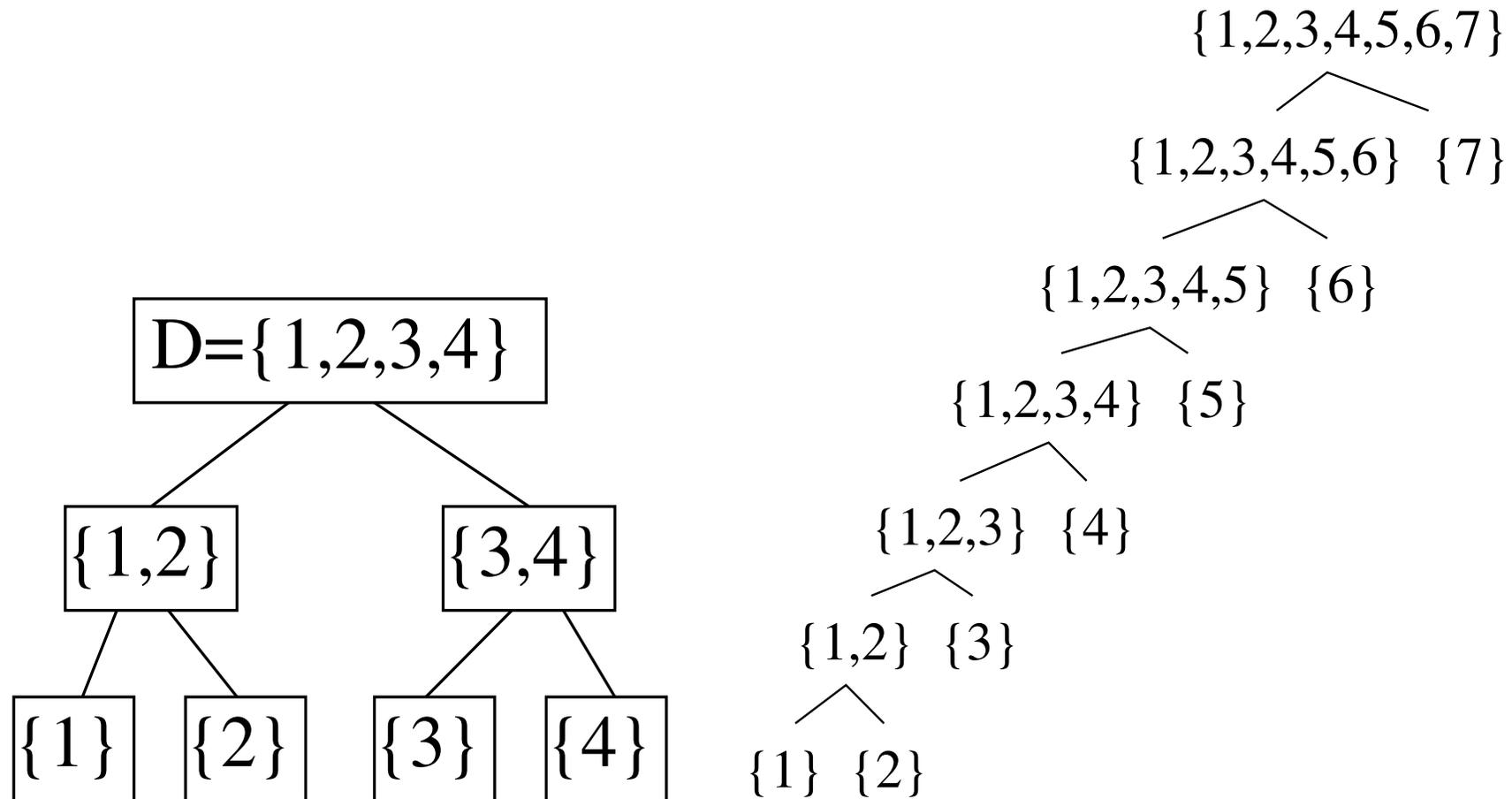


Figure 1: Balanced tree and linear tree

The hierarchical format based on the linear tree is also called the **TT format**.

3.2 Algorithmic Realisation

Typical situation: $U_{\{1,2\}} \subset U_1 \otimes U_2$ (nestedness property).

Bases: $U_1 = \text{span}_{1 \leq i \leq r_1} \{b_i^{(1)}\}$, $U_2 = \text{span}_{1 \leq j \leq r_2} \{b_j^{(2)}\}$, $U_{\{1,2\}} = \text{span}_{1 \leq \ell \leq r_{\{1,2\}}} \{b_\ell^{\{\{1,2\}\}}\}$.

$$b_\ell^{\{\{1,2\}\}} = \sum_{i=1}^{r_{\{1,2\}}} c_{ij}^{\{\{1,2\}, \ell\}} b_i^{(1)} \otimes b_j^{(2)}$$

Only the basis vectors $b_\nu^{(j)}$ of $U_j \subset V_j$ ($1 \leq j \leq d$) are explicitly stored,
for the other nodes store the coefficient matrices

$$C^{(\alpha, \ell)} = \left(c_{ij}^{(\alpha, \ell)} \right)_{ij} \in \mathbb{R}^{r_{\alpha_1} \times r_{\alpha_2}}.$$

The tensor is represented by $\mathbf{v} = c_1 b_1^{\{\{1, \dots, d\}\}}$.

Storage: $(d-1)r^3 + drn$ for $\left[C^{(\alpha, \ell)}, c_1, b_\nu^{(j)} \right]$ ($r := \max_\alpha \dim U_\alpha$; $n := \max_j \dim(V_j)$)

3.3 Operations - Example: scalar product

Let $\mathbf{v}, \mathbf{w} \in \mathbf{V}$ be given by the data $\left(C'(\alpha, \ell), c'_1, b_\nu'^{(j)}\right)$ and $\left(C''(\alpha, \ell), c''_1, b_\nu''(j)\right)$ resp.

$$\mathbf{v} = c'_1 \mathbf{b}_1'^{(D)}, \quad \mathbf{w} = c''_1 \mathbf{b}_1''(D) \quad \Rightarrow \quad \langle \mathbf{v}, \mathbf{w} \rangle = c'_1 c''_1 \left\langle \mathbf{b}_1'^{(D)}, \mathbf{b}_1''(D) \right\rangle.$$

Determine the scalar products $\beta_{ij}^{(\alpha)} := \left\langle \mathbf{b}_i'^{(\alpha)}, \mathbf{b}_j''(\alpha) \right\rangle$ recursively by

$$\begin{aligned} \beta_{ij}^{(\alpha)} &= \left\langle \mathbf{b}_i'^{(\alpha)}, \mathbf{b}_j''(\alpha) \right\rangle = \left\langle \sum_{k,\ell} c_{k,\ell}'^{(\alpha,i)} b_k'^{(\alpha_1)} \otimes b_\ell'^{(\alpha_2)}, \sum_{p,q} c_{p,q}''^{(\alpha,j)} b_p''(\alpha_1) \otimes b_q''(\alpha_2) \right\rangle \\ &= \sum_{k,\ell} \sum_{p,q} c_{k,\ell}'^{(\alpha,i)} c_{p,q}''^{(\alpha,j)} \left\langle b_k'^{(\alpha_1)}, b_p''(\alpha_1) \right\rangle \left\langle b_\ell'^{(\alpha_2)}, b_q''(\alpha_2) \right\rangle \\ &= \sum_{k,\ell} \sum_{p,q} c_{k,\ell}'^{(\alpha,i)} c_{p,q}''^{(\alpha,j)} \beta_{kp}^{(\alpha_1)} \beta_{lq}^{(\alpha_2)} \end{aligned}$$

$(\alpha_1, \alpha_2$: sons of α ; $\beta_{kp}^{(\alpha)}$ explicitly computable for leaves $\alpha = \{j\}$).

3.4 Basis Transformation

Set $\mathbf{B}_\alpha = [\mathbf{b}_1^{(\alpha)} \cdots \mathbf{b}_{r_\alpha}^{(\alpha)}]$. Let $\mathbf{B}'_\alpha = [\mathbf{b}'_1^{(\alpha)} \cdots \mathbf{b}'_{r_\alpha}^{(\alpha)}]$ be another basis.

The sons of α are denoted by α_1 and α_2 .

The relation

$$\mathbf{B}'_{\alpha_i} T^{(\alpha_i)} = \mathbf{B}_{\alpha_i} \quad (i = 1, 2)$$

corresponds to

$$C'(\alpha, \ell) = T^{(\alpha_1)} C(\alpha, \ell) (T^{(\alpha_2)})^\top \quad \text{for } 1 \leq \ell \leq r_\alpha.$$

Two directions:

1) Given \mathbf{B}_{α_i} , the new bases $\mathbf{B}'_{\alpha_i} := \mathbf{B}_{\alpha_i} (T^{(\alpha_i)})^{-1}$ lead to new coefficient matrices $C'(\alpha, \ell) := T^{(\alpha_1)} C(\alpha, \ell) (T^{(\alpha_2)})^\top$.

2) Given \mathbf{B}'_{α_i} and a decomposition $C'(\alpha, \ell) = T^{(\alpha_1)} \cdot C(\alpha, \ell) \cdot (T^{(\alpha_2)})^\top$, $C(\alpha, \ell)$ corresponds to $\mathbf{B}_{\alpha_i} := \mathbf{B}'_{\alpha_i} T^{(\alpha_i)}$.

3.5 Orthonormalisation

REMARK Let α be a vertex with sons α_1 and α_2 .

The basis $\{\mathbf{b}_\ell^{(\alpha)}\}$ is orthonormal, if

(a) the bases $\{\mathbf{b}_i^{(\alpha_1)}\}$ and $\{\mathbf{b}_j^{(\alpha_2)}\}$ of the sons are orthonormal and

(b) the matrices $C^{(\alpha,\ell)}$ are orthonormal with respect to the Frobenius scalar product:

$$\langle C^{(\alpha,\ell)}, C^{(\alpha,m)} \rangle_{\text{F}} = \sum_{ij} \langle c_{ij}^{(\alpha,\ell)}, c_{ij}^{(\alpha,m)} \rangle = \delta_{\ell m}.$$

Algorithm:

(a) Orthonormalise the explicitly given bases at the leaves (e.g., by QR).

(b) As soon as $\{\mathbf{b}_i^{(\alpha_1)}\}$ and $\{\mathbf{b}_j^{(\alpha_2)}\}$ are orthonormal, orthonormalise the matrices $\{C^{(\alpha,\ell)}\}$.

The new matrices $C_{\text{new}}^{(\alpha,\ell)}$ define the new orthonormal basis $\{\mathbf{b}_{\ell,\text{new}}^{(\alpha)}\}$.

3.6 HOSVD and HOSVD Bases

We recall: The HOSVD basis $\{\mathbf{b}_\ell^{(\alpha)}\}$ consists of the normalised eigenvectors of $M_\alpha M_\alpha^\top$, where $M_\alpha := \mathcal{M}_\alpha(\mathbf{v})$ is the α -matricisation of the tensor \mathbf{v} .

Instead of $\{\mathbf{b}_\ell^{(\alpha)}\}$ we need the corresponding coefficient matrices $\{C_{\text{HOSVD}}^{(\alpha,\ell)}\}$.

Step 1: Orthonormalisation of the bases.

Step 2: Recursion from the root to the leaves:

2a) Start at the root: $\sigma_1^{(\text{root})} := |c_1^{(\text{root})}|$ where $\mathbf{v} = c_1^{(\text{root})} \mathbf{b}_1^{(\text{root})}$.

2b) Set

$$E_{\alpha_1} := \sum_{i=1}^{r_\alpha} (\sigma_i^{(\alpha)})^2 C^{(\alpha,i)} (C^{(\alpha,i)})^H, \quad E_{\alpha_2} := \sum_{i=1}^{r_\alpha} (\sigma_i^{(\alpha)})^2 ((C^{(\alpha,i)})^H C^{(\alpha,i)})^\top.$$

Diagonalisation yields

$$E_{\alpha_1} = U \Sigma_{\alpha_1}^2 U^H, \quad E_{\alpha_2} = V \Sigma_{\alpha_2}^2 V^H \quad \text{with} \quad \Sigma_{\alpha_i} = \text{diag}\{\sigma_\nu^{(\alpha_i)}\}.$$

$\mathbf{B}_{\alpha_1}^{\text{HOSVD}} := \mathbf{B}_{\alpha_1} U$ and $\mathbf{B}_{\alpha_2}^{\text{HOSVD}} = \mathbf{B}_{\alpha_2} V$ are the desired HOSVD bases.

Arithmetical cost: $O(dr^4 + dnr^2)$.

3.7 HOSVD Truncation

Represent the tensor \mathbf{v} with respect to the HOSVD bases $\left\{ b_\ell^{(\alpha)} : 1 \leq \ell \leq r_\alpha \right\}$.

Choose smaller dimensions

$$s_\alpha \leq r_\alpha.$$

Omit all terms corresponding to $\left\{ b_\ell^{(\alpha)} : s_\alpha < \ell \leq r_\alpha \right\}$. Result: $\mathbf{v}_{\text{HOSVD}}$.

Then the following estimates hold:

$$\|\mathbf{v} - \mathbf{v}_{\text{HOSVD}}\| \leq \left(\sum_{\alpha} \sum_{\nu \geq s_\alpha + 1} (\sigma_\nu^{(\alpha)})^2 \right)^{1/2} \leq (2d - 3)^{1/2} \|\mathbf{v} - \mathbf{v}_{\text{best}}\|.$$

4 Solution of Linear Systems

Linear system

$$\mathbf{Ax} = \mathbf{b},$$

where $\mathbf{x}, \mathbf{b} \in \mathbf{V} = \bigotimes_{j=1}^d V_j$ and $\mathbf{A} \in \bigotimes_{j=1}^d \mathcal{L}(V_j, V_j) \subset \mathcal{L}(\mathbf{V}, \mathbf{V})$ are represented in one of the formats (e.g., \mathbf{A} : r -term format, \mathbf{x}, \mathbf{b} : hierarchical format):

Standard linear iteration:

$$\mathbf{x}^{m+1} = \mathbf{x}^m - \mathbf{B}(\mathbf{Ax}^m - \mathbf{b}).$$

\Rightarrow representation ranks blow up.

Therefore truncations T are used ('truncated iteration'):

$$\mathbf{x}^{m+1} = T(\mathbf{x}^m - \mathbf{B}(T(\mathbf{Ax}^m - \mathbf{b}))).$$

Cost per step: $nd \times$ powers of the involved representation ranks.

$$\mathbf{x}^{m+1} = T(\mathbf{x}^m - \mathbf{B}(T(\mathbf{A}\mathbf{x}^m - \mathbf{b})))$$

Choice of \mathbf{B} :

If \mathbf{A} corresponds to an elliptic pde of order 2, the discretisation of Δ is spectrally equivalent $\Rightarrow \mathbf{B} = \mathbf{B}_r$ from above has a simple r -term format.

Obvious variants: cg-like methods

Literature:

Khoromskij 2009, Kressner-Tobler 2010, Kressner-Tobler 2011 (SIAM),
Kressner-Tobler 2011 (CMAM), Osedelets-Tyrtysnikov-Zamarashkin 2011,
Ballani-Grasedyck 2013, Savas-Eldén 2013

Remark: For $d = 2$, these linear systems may be written as matrix equations:

$$(A \otimes I + I \otimes A) \mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad AX + XA = B \quad (\text{Lyapunov})$$

(cf. Benner-Breiten 2013).

5 Variational Approach

Define

$$\Phi(\mathbf{x}) := \langle \mathbf{Ax}, \mathbf{x} \rangle - 2 \langle \mathbf{b}, \mathbf{x} \rangle$$

if \mathbf{A} is positive definite or

$$\Phi(\mathbf{x}) := \|\mathbf{Ax} - \mathbf{b}\|^2$$

or

$$\Phi(\mathbf{x}) := \|\mathbf{B}(\mathbf{Ax} - \mathbf{b})\|^2$$

and try to minimise $\Phi(\mathbf{x})$ over all parameters of \mathbf{x} in a fixed format.

Literature:

Espig-Hackbusch-Rohwedder-Schneider, Falcó-Nouy,
Holtz-Rohwedder-Schneider, Mohlenkamp, Osedelets,...

5.1 Formulation of the Problem, ALS Method

Let

$$\Phi(\mathbf{u}) = \min$$

be a minimisation problem over the whole tensor space $\mathbf{u} \in \mathbf{V}$.

Approximation: Choose any format $\mathcal{F} \subset \mathbf{V}$. Solve

$$\Phi(\mathbf{u}) = \min \text{ over all } \mathbf{v} \in \mathcal{F}.$$

This is the minimisation over all parameters in the representation of $\mathbf{v} \in \mathcal{F}$.

Difficulty: While the original problem may be convex, the new problem is not.

Example: $\Phi(\mathbf{u}) = \|\mathbf{v} - \mathbf{u}\|^2$ over all $\mathbf{u} \in \mathcal{R}_1 = \mathcal{I}_{(1,\dots,1)}$. $\mathbf{v} \in \mathbf{V}$ is arbitrary.

Ansatz:

$$\mathbf{u} = u^{(1)} \otimes u^{(2)} \otimes \dots \otimes u^{(d)}, \quad u^{(j)} \in V_j = \mathbb{R}^{n_j}$$

Necessary condition: $\nabla\Phi(\mathbf{u}) = 0$ (multilinear system of equations).

ALS = alternating least-squares method:

1) solve $\nabla\Phi(u^{(1)} \otimes u^{(2)} \otimes \dots \otimes u^{(d)}) = 0$ w.r.t. $u^{(1)} \Rightarrow$ solution: $\hat{u}^{(1)}$,

2) solve $\nabla\Phi(\hat{u}^{(1)} \otimes u^{(2)} \otimes \dots \otimes u^{(d)}) = 0$ w.r.t. $u^{(2)} \Rightarrow$ solution: $\hat{u}^{(2)}$,

⋮

d) solve $\nabla\Phi(\hat{u}^{(1)} \otimes \dots \otimes \hat{u}^{(d-1)} \otimes u^{(d)}) = 0$ w.r.t. $u^{(d)} \Rightarrow$ solution: $\hat{u}^{(d)}$

All partial steps are **linear problems** and easy to solve.

One ALS iteration is given by $\mathbf{u}_0 = u^{(1)} \otimes \dots \otimes u^{(d)} \mapsto \mathbf{u}_1 = \hat{u}^{(1)} \otimes \dots \otimes \hat{u}^{(d)}$.

This defines a ALS sequence $\{\mathbf{u}_m : m \in \mathbb{N}_0\}$.

Questions: Does \mathbf{u}_m converge? To what limit? Convergence speed?

5.2 First Results

Mohlenkamp (2013, Linear Algebra Appl. 438):

- The sequence $\{\mathbf{u}_m : m \in \mathbb{N}_0\}$ is bounded,
- $\|\mathbf{u}_m - \mathbf{u}_{m+1}\| \rightarrow 0$,
- $\sum_{m=0}^{\infty} \|\mathbf{u}_m - \mathbf{u}_{m+1}\|^2 < \infty$,
- the set S of accumulation points of $\{\mathbf{u}_m\}$ is connected and compact.

Conclusion: If S contains an isolated point \mathbf{u}^* , it follows that $\mathbf{u}_m \rightarrow \mathbf{u}^*$.

Note that, in general, the limit may depend on the starting value!

5.3 Study of Examples

5.3.1 Case of $d = 2$

$$\mathbf{v} := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \Phi(\mathbf{u}) = \|\mathbf{v} - \mathbf{u}\|^2.$$

1) $\mathbf{u}^{**} = 2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is the global minimiser and an attractive fixed point.

2) $\mathbf{u}^* = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is a fixed point of the ALS iteration:

$$\Phi(\mathbf{u}^* + \delta_1 \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}) = \Phi(\mathbf{u}^*) + \|\delta_1\|^2.$$

$$\text{But } \Phi\left(\begin{pmatrix} 1 \\ t \end{pmatrix} \otimes \begin{pmatrix} 1 \\ t \end{pmatrix}\right) = \Phi(\mathbf{u}^*) - t^2(2 - t^2)$$

$\Rightarrow \mathbf{u}^*$ is a saddle point and a repulsive fixed point.

Conclusion: Almost all starting values lead to $\mathbf{u}_m \rightarrow \mathbf{u}^{**}$.

5.3.2 Case of $d \geq 3$

For $a \perp b$ with $\|a\| = \|b\| = 1$ consider $\Phi(\mathbf{u}) = \|\mathbf{v} - \mathbf{u}\|^2$ with

$$\mathbf{v} = \otimes^3 a + 2 \otimes^3 b.$$

Again $\mathbf{u}^* = \otimes^3 a$ and $\mathbf{u}^{**} = 2 \otimes^3 b$ are fixed points, $\Phi(\mathbf{u}^{**}) < \Phi(\mathbf{u}^*)$.

But now **both are local minima** (attractive fixed points)!

Additional **saddle point** (repulsive fixed point): $\mathbf{u}^{***} = c \otimes^3 (a + \frac{1}{2}b)$.

The sequence $\{\mathbf{u}_m\}$ corresponding to the starting value

$$\mathbf{u}_0 = c^{(0)} \left(a + t_1^{(0)} b \right) \otimes \left(a + t_2^{(0)} b \right) \otimes \left(a + t_3^{(0)} b \right)$$

is completely defined by $t_2^{(0)}$ and $t_3^{(0)}$. The characteristic value is

$$\tau_m := \left| t_2^{(m)} \right|^\alpha \left| t_3^{(m)} \right|^\beta \quad \text{with} \quad \alpha = 5^{1/2} - 1, \quad \beta = 2.$$

(A) $\tau_0 > 2^{-\gamma}$, $\gamma = 5^{1/2} + 1 \Rightarrow \mathbf{u}_m \rightarrow \mathbf{u}^{**}$ (global minimiser),

(B) $\tau_0 < 2^{-\gamma} \Rightarrow \mathbf{u}_m \rightarrow \mathbf{u}^*$ (local minimiser),

(C) $\tau_0 = 2^{-\gamma} \Rightarrow \mathbf{u}_m \rightarrow \mathbf{u}^{***}$ (saddle point, global minimiser on the manifold $\tau = 2^{-\gamma}$).

We recall:

Conclusion: If the set of accumulation points of $\{\mathbf{u}_m\}$ contains an isolated point \mathbf{u}^* , it follows that $\mathbf{u}_m \rightarrow \mathbf{u}^*$.

Wang–Chu (2014): Global convergence for almost all \mathbf{u}_0 .

Uschmajew (2015):

Analysis based on the Łojasiewicz inequality yields:

All sequences \mathbf{u}_m converge to some \mathbf{u}^* with $\nabla\Phi(\mathbf{u}^*) = 0$.

Łojasiewicz (1965, Ensembles semi-analytiques): If Φ is analytic,

$$\exists\theta \in (0, 1/2] \quad |\Phi(x) - \Phi(x_*)|^{1-\theta} \leq \|\nabla\Phi(x)\|$$

in some neighbourhood of x_* .

Convergence speed?

The proof by the Łojasiewicz inequality is not constructive.

Espig–Khachatryan (2015): Study of sequences for $\Phi(\mathbf{u}) = \|\mathbf{v} - \mathbf{u}\|^2$ with

$$\begin{aligned} \mathbf{v} &= \otimes^3 a + \lambda (a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a), \\ a \perp b, \quad \|a\| &= \|b\| = 1. \end{aligned}$$

Depending on the value of λ it is shown that the convergence can be

- sublinear ($\lambda = 1/2$),
- linear ($\lambda < 1/2$).

For $\mathbf{v} = \otimes^3 a + 2 \otimes^3 b$, $\mathbf{u}_m \rightarrow \otimes^3 a$ or $2 \otimes^3 b$, we have

- superlinear convergence (of order $2 + 5^{1/2} > 1$)

Study of the general case: Gong–Mohlenkamp–Young 2017

6 Multivariate Cross Approximation

Matrix Case

Problem: given $M \in \mathbb{K}^{I \times J}$, find a rank- r matrix R_r close to M evaluating only $O(r(\#I + \#J))$ entries.

Choose r rows (index subset $\tau := \{i_1, \dots, i_r\} \subset I$) and r columns (index subset $\sigma := \{j_1, \dots, j_r\} \subset J$).

$$M = \begin{bmatrix} & * & & * & & * & & & & & \\ & * & & * & & * & & & & & \\ * & * & * & * & * & * & * & * & * & * & * \\ & * & & * & & * & & & & & \\ * & * & * & * & * & * & * & * & * & * & * \\ & * & & * & & * & & & & & \\ * & * & * & * & * & * & * & * & * & * & * \\ & * & & * & & * & & & & & \\ & * & & * & & * & & & & & \end{bmatrix}$$

Then, a matrix R_r of rank r with

$$R[i, j] = M[i, j] \quad \text{for all index pairs with either } i \in \tau \text{ or } j \in \sigma$$

is given by

$$R_r = M|_{I \times \sigma} \cdot (M|_{\tau \times \sigma})^{-1} \cdot M|_{\tau \times J},$$

provided that the $r \times r$ matrix $M|_{\tau \times \sigma}$ is regular.

$$M = \begin{bmatrix} * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \\ * & * & * & * & * & * & * & * & * & * \end{bmatrix}$$

If $\text{rank}(M) = r$, there exist subsets τ, σ such that $M|_{\tau \times \sigma}$ is regular and $R_r = M$.

Adaptive Cross Approximation (ACA): adaptive choice of τ, σ .

Generalisation to order $d \geq 3$

- hierarchical format
- Apply the previous idea to all matricisations

$$M := \mathcal{M}_\alpha(\mathbf{v}).$$

- M is large, but the matrix $(M|_{\tau \times \sigma})^{-1}$ is still of size $r \times r$.

Then:

Required number of evaluations of the tensor is $O\left(\sum_j \#I_j\right)$.

If \mathbf{v} has hierarchical rank $\mathfrak{r} := (\text{rank}_\alpha(\mathbf{v}))_{\alpha \in T_D}$, it can be reconstructed in $\mathcal{H}_{\mathfrak{r}}$ exactly.

Suited for applications to multivariate functions.

EXAMPLE: Approximation of a special multilinear function

Boundary-element application. Solution of $-\Delta u = 0$ in $\Omega \subset \mathbb{R}^3$ with boundary Γ . Ansatz functions: piecewise constant functions for a triangulation \mathcal{T} .

Galerkin matrix:

$$M_{\Delta' \Delta''} = \iint_{\Delta'} \iint_{\Delta''} \frac{d\Gamma_{\mathbf{x}} d\Gamma_{\mathbf{y}}}{\|\mathbf{x} - \mathbf{y}\|} \quad (\Delta', \Delta'' \in \mathcal{T}).$$

Difficult cases: $\Delta' \cap \Delta'' \neq \emptyset$.

Case of one common side.

W.l.o.g. the corners of Δ' are $(0, 0, 0)$, $(1, 0, 0)$, $(x, y, 0)$, while those of Δ'' are $(0, 0, 0)$, $(1, 0, 0)$, (ξ, η, τ) .

$$\Rightarrow M_{\Delta' \Delta''} = f(x, y, \xi, \eta, \tau).$$

Tensor approximation faster than quadrature by a factor of 630 to 2800 (cf. Ballani 2012).

7 PDEs with stochastic coefficients

Literature: Espig-Hackbusch-Litvinenko-Matthies-Wöhnert: *Efficient low-rank approximation of the stochastic Galerkin matrix in tensor formats*. Comput. Math. Appl. **67** (2014) 818–829

7.1 Formulation of the problem

Boundary value problem in $D \subset \mathbb{R}^d$ ($1 \leq d \leq 3$):

$$\begin{aligned} \operatorname{div} \kappa(x, \omega) \operatorname{grad} u &= f \quad \text{for } x \in D, \omega \in \Omega, \\ u &= 0 \quad \text{on } \partial D. \end{aligned}$$

Assumption (log-normal distribution):

$$\kappa(x, \omega) = \exp(\gamma(x, \omega)), \quad \gamma \text{ Gaussian random field.}$$

Solution $u = u(x, \omega) \in L^2(\Omega, H_0^1(D))$.

Weak formulation: $a(u, v) = f(v)$ for all $v \in L^2(\Omega, H_0^1(D))$.

Stochastic quantities:

Mean functions:

$$m_{\kappa}(x) := \mathbb{E}(\kappa(x, \cdot)),$$

$$m_{\gamma}(x) := \mathbb{E}(\gamma(x, \cdot)),$$

covariance functions:

$$\Gamma_{\kappa}(x, y) := \mathbb{E}[(\kappa(x, \cdot) - m_{\kappa}(x))(\kappa(y, \cdot) - m_{\kappa}(y))],$$

$$\Gamma_{\gamma}(x, y) := \mathbb{E}[(\gamma(x, \cdot) - m_{\gamma}(x))(\gamma(y, \cdot) - m_{\gamma}(y))].$$

Interconnection:

$$m_{\gamma}(x) = 2 \log m_{\kappa}(x) - \frac{1}{2} \log (\Gamma_{\kappa}(x, x) + m_{\kappa}(x)^2),$$

$$\Gamma_{\gamma}(x, y) = \log \left(1 + \frac{\Gamma_{\kappa}(x, y)}{m_{\kappa}(x)m_{\kappa}(y)} \right).$$

Singular value decompositions (sums restricted to positive singular values):

$$\tilde{\kappa}(x, \omega) := \kappa(x, \omega) - m_\kappa(x) = \sum_k (\lambda_k)^{1/2} \kappa_k(x) \Phi_k(\omega),$$

$$\tilde{\gamma}(x, \omega) := \gamma(x, \omega) - m_\gamma(x) = \sum_k (\lambda'_k)^{1/2} \gamma_k(x) \theta_k(\omega).$$

The $L^2(D)$ orthonormal system $\{\kappa_k\}$ are the eigenfunctions of the Hilbert-Schmidt operator

$$C_\kappa \in \mathcal{L}(L^2(D), L^2(D)), \quad (C_\kappa \varphi)(x) = \int_D \Gamma_\kappa(x, y) \varphi(y) dy,$$

$$C_\kappa \kappa_k = \lambda_k \kappa_k.$$

Similarly,

$$C_\gamma \in \mathcal{L}(L^2(D), L^2(D)), \quad (C_\gamma \varphi)(x) = \int_D \Gamma_\gamma(x, y) \varphi(y) dy,$$

$$C_\gamma \gamma_k = \lambda'_k \gamma_k.$$

Furthermore,

$$\theta_k(\omega) = (\lambda'_k)^{-1/2} \int_D [\gamma(x, \omega) - m_\gamma(x)] \gamma_k(x) dx$$

are jointly normal distributed and orthonormal random variables in $L^2(\Omega)$.

Uniform ellipticity:

In the following, we assume that

$$\sum_k (\lambda'_k)^{1/2} \|\gamma_k\|_\infty < \infty.$$

Then one can show that

$$0 < \underline{\kappa} \leq \kappa(x, \omega)$$

holds almost surely and for almost all $x \in D$.

Consequence: Sufficiently small perturbations of $\kappa(x, \omega)$ do not change the ellipticity of the problem.

Multivariate Hermite polynomials $L^2(\Omega)$:

$$H_{\boldsymbol{\nu}}(\mathbf{x}) := \prod_{k=1}^{\infty} h_{\nu_k}(x_k) \quad \text{for } \boldsymbol{\nu} \in \ell_0(\mathbb{N});$$

h_i : i -th Hermite polynomial,

$$\ell_0(\mathbb{N}) := \{\boldsymbol{\nu} = (\nu_k)_{k \in \mathbb{N}} : \nu_k \in \mathbb{N}_0, \nu_k = 0 \text{ for almost all } k \in \mathbb{N}\};$$

Set

$$\boldsymbol{\theta} = (\theta_k)_{k \in \mathbb{N}} \text{ orthonormal system in } L^2(\Omega).$$

Then $\{(\boldsymbol{\nu}!)^{-1/2} H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) : \boldsymbol{\nu} \in \ell_0(\mathbb{N})\}$ is an orthonormal basis in $L^2(\Omega)$ and

$$\mathbb{E} \left(\kappa(x, \cdot) (\boldsymbol{\nu}!)^{-1/2} H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) \right) = m_{\kappa}(x) \prod_k \left((\lambda'_k)^{1/2} \gamma_k(x) \right)^{\nu_k} (\nu_k!)^{-1/2}$$

(cf. Janson: Gaussian Hilbert Spaces, 1997; Ullmann: PhD thesis 2008).

The expansion of

$$\tilde{\kappa} = \kappa - m_\kappa = \sum_{\nu \in \ell_0(\mathbb{N})} \sum_{\ell \in \mathbb{N}} \xi_\ell^{(\nu)} (\nu!)^{-1/2} \kappa_\ell \otimes H_\nu(\boldsymbol{\theta}) \in L^2(D \times \Omega)$$

into the orthonormal basis

$$\left\{ (\nu!)^{-1/2} \kappa_\ell \otimes H_\nu(\boldsymbol{\theta}) : \nu \in \ell_0(\mathbb{N}), \ell \in \mathbb{N} \right\}$$

has the coefficients

$$\begin{aligned} \xi_{\ell, \nu} &= (\nu!)^{-1/2} \int_D \kappa_\ell(x) \mathbb{E} [\kappa(x, \cdot) H_\nu(\boldsymbol{\theta})] dx \\ &= \int_D \kappa_\ell(x) m_\kappa(x) \prod_k \left((\lambda'_k)^{1/2} \gamma_k(x) \right)^{\nu_k} (\nu_k!)^{-1/2} dx \\ &\quad - \delta_{0\nu} \int_D \kappa_\ell(x) m_\kappa(x) dx \end{aligned}$$

($\delta_{0\nu}$: Kronecker delta).

7.2 Discretisation

Spatial discretisation: subspace $V_N \subset H_0^1(D)$ spanned by

$$\{\varphi_1, \dots, \varphi_N\}.$$

Stochastic discretisation: subspace $S_J \subset L^2(\Omega)$ spanned by

$$\{H_\iota(\boldsymbol{\theta}) : \iota \in J\} \quad \text{with} \quad \#J < \infty, \quad p_k = \max\{\iota_k : \iota \in J\}.$$

Galerkin discretisation:

$$\begin{aligned} & a(\varphi_i \otimes H_\alpha(\boldsymbol{\theta}), \varphi_j \otimes H_\beta(\boldsymbol{\theta})) \\ = & \delta_{\alpha\beta} \int_D m_\kappa(x) \langle \nabla \varphi_i(x), \nabla \varphi_j(x) \rangle dx \\ & + \sum_{\ell=1}^{\infty} \xi_\ell^{(\iota)} \cdot \mathbb{E}(H_\iota(\boldsymbol{\theta}) H_\alpha(\boldsymbol{\theta}) H_\beta(\boldsymbol{\theta})) \cdot \int_D \kappa_\ell(x) \langle \nabla \varphi_i(x), \nabla \varphi_j(x) \rangle dx \end{aligned}$$

Stochastic Galerkin matrix:

$$\begin{aligned} \mathbf{K} &:= \left(a(\varphi_i \otimes H_\alpha, \varphi_j \otimes H_\beta) \right)_{(i,\alpha),(j,\beta)} \\ &= K_0 \otimes \Delta_0 + \sum_{\ell} \sum_{\iota \in J} \xi_{\ell}^{(\iota)} K_{\ell} \otimes \bigotimes_{k=1}^K \Delta_{\iota_k} \in \mathbb{R}^{N \times N} \otimes \bigotimes_{k=1}^K \mathbb{R}^{(p_k+1) \times (p_k+1)} \end{aligned}$$

with

$$\begin{aligned} K &:= \max\{k : \iota_k > 0 \text{ for some } \iota \in J\}, \\ (\Delta_{\iota_k})_{\alpha\beta} &:= \mathbb{E}(H_{\iota_k}(\theta_k) H_{\alpha}(\theta_k) H_{\beta}(\theta_k)), \quad \Delta_{\iota_k} \in \mathbb{R}^{(p_k+1) \times (p_k+1)}, \\ (K_{\ell})_{ij} &:= \int_D \kappa_{\ell}(x) \langle \nabla \varphi_i(x), \nabla \varphi_j(x) \rangle dx, \quad K_{\ell} \in \mathbb{R}^{N \times N}, \\ (K_0)_{ij} &:= \int_D m_{\kappa}(x) \langle \nabla \varphi_i(x), \nabla \varphi_j(x) \rangle dx, \quad K_0 \in \mathbb{R}^{N \times N}. \end{aligned}$$

The size of the stochastic Galerkin matrix is

$$\left(N \cdot \prod_{k=1}^K (p_k + 1) \right) \times \left(N \cdot \prod_{k=1}^K (p_k + 1) \right).$$

Truncation of $\ell \in \mathbb{N}$ in

$$\mathbf{K} = K_0 \otimes \Delta_0 + \sum_{\ell \in \mathbb{N}} \sum_{\iota \in J} \xi_\ell^{(\iota)} K_\ell \otimes \bigotimes_{k=1}^K \Delta_{\iota_k}$$

to $\ell \in \{1, \dots, M\}$ yields a finite expression

$$\mathbf{K} \approx \mathbf{L} := K_0 \otimes \Delta_0 + \sum_{\ell=1}^M \sum_{\iota \in J} \xi_\ell^{(\iota)} K_\ell \otimes \bigotimes_{k=1}^K \Delta_{\iota_k}.$$

The approximation error is proportional to $\sum_{\ell=M+1}^{\infty} \lambda_\ell \rightarrow 0$.

Question: What is a suitable representation of the huge matrix \mathbf{L} or its approximation?

Later numerical example:

$$N = 1000, p = 10, K = 20 \quad \Rightarrow \quad N \cdot (p + 1)^{20} \approx 6.7 \times 10^{23}.$$

7.3 Tensor rank of the stochastic Galerkin matrix

$1 + M \cdot \#J$ terms are involved in

$$\mathbf{L} := K_0 \otimes \Delta_0 + \sum_{\ell=1}^M \sum_{\iota \in J} \xi_{\ell, \iota} K_\ell \otimes \bigotimes_{k=1}^K \Delta_{\iota_k}.$$

Assume that we can approximate the tensor

$$\xi \in \mathbb{R}^M \otimes \bigotimes_{k=1}^K \mathbb{R}^{p_k+1}$$

by η in R -term format: $\eta = \sum_{j=1}^R \left[y_j^{(0)} \otimes \bigotimes_{k=1}^K y_j^{(k)} \right]$; i.e.,

$$\eta_{\ell, \iota} = \sum_{j=1}^R \left[\left(y_j^{(0)} \right)_\ell \cdot \prod_{k=1}^K \left(y_j^{(k)} \right)_{\iota_k} \right] \quad \text{with } y_j^{(0)} \in \mathbb{R}^M \text{ and } y_j^{(k)} \in \mathbb{R}^{p_k+1}.$$

Then

$$\hat{\mathbf{L}} = K_0 \otimes \Delta_0 + \sum_{j=1}^R \left(\sum_{\ell=1}^M \left(y_j^{(0)} \right)_\ell K_\ell \right) \otimes \bigotimes_{k=1}^K \left(\sum_{\iota_k} \left(y_j^{(k)} \right)_{\iota_k} \Delta_{\iota_k} \right),$$

i.e., $\hat{\mathbf{L}}$ has an $(1 + R)$ -term representation: $\hat{\mathbf{L}} \in \mathcal{R}_{1+R}$.

\Rightarrow also the other ranks (Tucker, hierarchical format, TT) are $\leq 1 + R$.

Interludio:

$$V_j = \mathbb{K}^{I_j}, \quad \mathbf{V} = \bigotimes_j V_j.$$

For each $i_j \in I_j$ is associated to a function $f_{i_j}^{(j)}$.

The tensor $\mathbf{v} \in \mathbf{V}$ is defined by

$$\mathbf{v}[i_1, \dots, i_d] = \int_D \prod_{j=1}^d f_{i_j}^{(j)}(x) dx.$$

Then quadrature yields

$$\mathbf{v}[i_1, \dots, i_d] \approx \tilde{\mathbf{v}}[i_1, \dots, i_d] := \sum_{\ell=1}^R \omega_\ell \prod_{j=1}^d f_{i_j}^{(j)}(x_\ell).$$

Set $v_\ell^{(j)} := \left(f_{i_j}^{(j)}(x_\ell) \right)_{i_j \in I_j} \in V_j$. Then $\tilde{\mathbf{v}}[i_1, \dots, i_d] = \sum_{\ell=1}^R \omega_\ell \prod_{j=1}^d v_\ell^{(j)}[i_j]$,

i.e.,

$$\tilde{\mathbf{v}} = \sum_{\ell=1}^R \omega_\ell \bigotimes_{j=1}^d v_\ell^{(j)} \in \mathcal{R}_R.$$

Explicit description of ξ :

$$\xi_{\ell, \iota} := \int_D \kappa_\ell(x) m_\kappa(x) \prod_{k=1}^K \left\{ \left[(\lambda'_k)^{\frac{1}{2}} \gamma_k(x) \right]^{\iota_k} (\iota_k!)^{-\frac{1}{2}} \right\} dx - \delta_{0, \iota} \int_D \kappa_\ell(x) m_\kappa(x) dx.$$

Apply a quadrature to $\int_D \cdots dx$: $\xi_{\ell, \iota} \approx \eta_{\ell, \iota} :=$

$$\sum_{j=1}^R \omega_j \kappa_\ell(x_j) m_\kappa(x_j) \prod_{k=1}^K \left\{ \left[(\lambda'_k)^{1/2} \gamma_k(x_j) \right]^{\iota_k} (\iota_k!)^{-1/2} \right\} - \delta_{0, \iota} \sum_{j'=1}^R \omega_{j'} \kappa_\ell(x_{j'}) m_\kappa(x_{j'}).$$

This yields the desired $(R + 1)$ -term representation of η :

$$\begin{aligned} \left(y_j^{(0)} \right)_\ell &:= \omega_j \kappa_\ell(x_j) m_\kappa(x_j), \\ \left(y_j^{(k)} \right)_{\iota_k} &:= \left[(\lambda'_k)^{1/2} \gamma_k(x_j) \right]^{\iota_k} (\iota_k!)^{-1/2} \quad (1 \leq k \leq K) \end{aligned}$$

for $1 \leq j \leq R$.

The additional term for $j = 0$ is

$$\left(y_0^{(0)} \right)_\ell := - \sum_{j'=1}^R \omega_{j'} \kappa_\ell(x_{j'}) m_\kappa(x_{j'}), \quad \left(y_0^{(k)} \right)_{\iota_k} := \delta_{0, \iota_k}.$$

The error $\|\xi - \eta\|_F$ (quadrature error) does not depend on J (i.e., on K and p_k).

Final problem:

$$\hat{\mathbf{L}}\mathbf{u} = \left(\sum_{j=0}^R \hat{K}_j \otimes \hat{\Delta}_j \right) \mathbf{u} = \mathbf{f}.$$

Let B the approximate inverse of the discrete Laplacian. Then

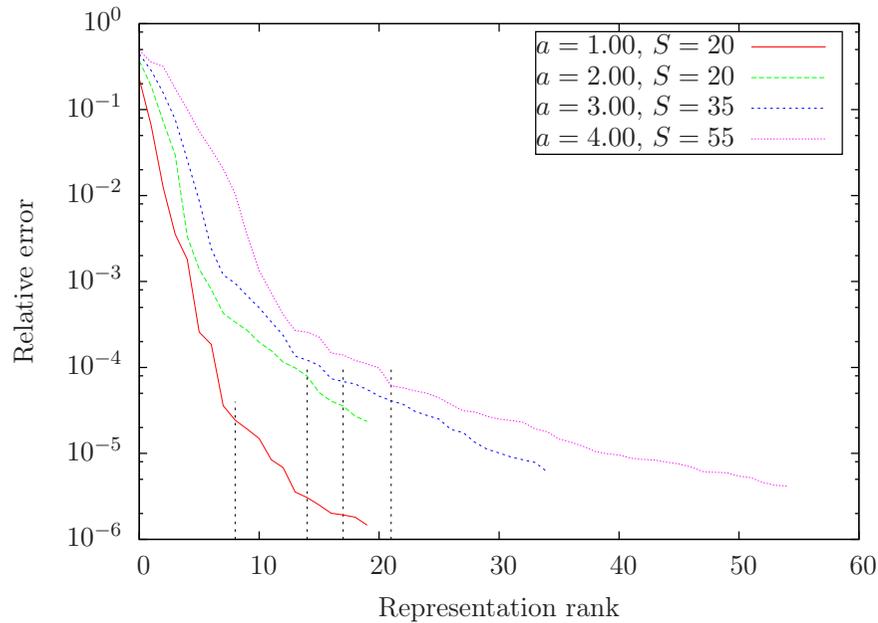
$$\sigma(B\hat{K}_j) = O(1)$$

and $(B \otimes I)\hat{\mathbf{L}}$ is well-conditioned.

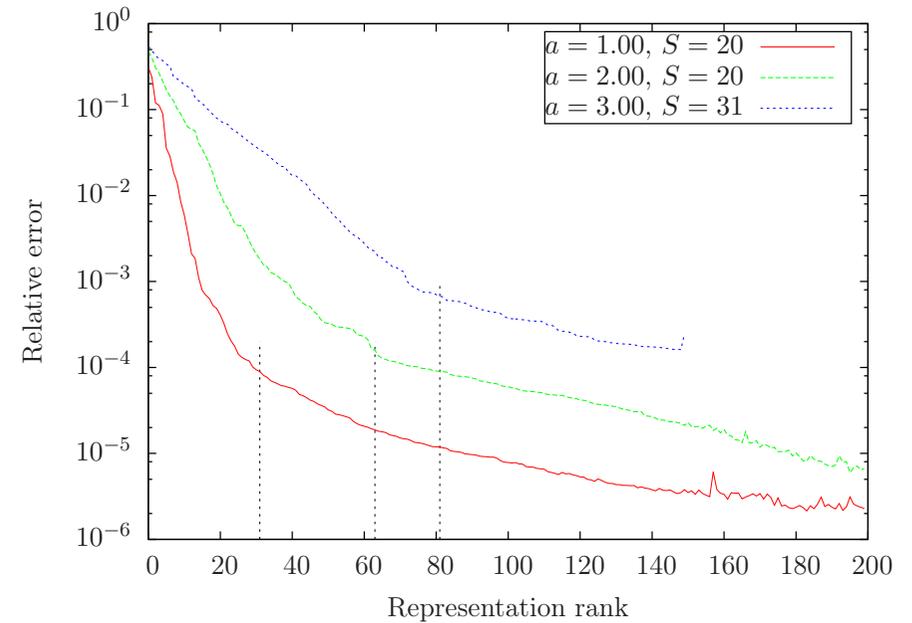
Numerical results with

$$\Gamma_{\kappa}(x, y) = \exp(-a^2 \|x - y\|^2), \quad \frac{1}{a} \text{ covariance length,}$$

Gaussian quadrature with S points per direction:



$$D = (0, 1)$$



$$D = (0, 1)^2$$

8 Minimal Subspaces

8.1 Definitions

We recall the definition of the **algebraic tensor space**:

$$\mathbf{V} := \text{span} \left\{ \bigotimes_{j=1}^d v^{(j)} : v^{(j)} \in V_j \right\} =: \bigotimes_{j=1}^d V_j$$

Here, $\dim(V_j) = \infty$ may hold.

Question: Given $\mathbf{v} \in \mathbf{V}$, are there minimal subspaces $U_j^{\min}(\mathbf{v}) \subset V_j$ such that

$$\mathbf{v} \in \bigotimes_{j=1}^d U_j^{\min}(\mathbf{v}),$$

$$\mathbf{v} \in \bigotimes_{j=1}^d U_j \implies U_j^{\min}(\mathbf{v}) \subset U_j.$$

Such subspaces are the optimal choice for the tensor subspace representation (Tucker).

Elementary results:

- 1) There are finite-dimensional U_j with $\mathbf{v} \in \bigotimes_{j=1}^d U_j$, more precisely $\dim(U_j) \leq \text{rank}(\mathbf{v})$.
- 2) $\mathbf{v} \in \bigotimes_{j=1}^d U_j'$ and $\mathbf{v} \in \bigotimes_{j=1}^d U_j''$ imply $\mathbf{v} \in \bigotimes_{j=1}^d (U_j' \cap U_j'')$.
- 3) The intersection of all U_j with $\mathbf{v} \in \bigotimes_{j=1}^d U_j$ yields $U_j^{\min}(\mathbf{v})$.

Characterisation of $U_j^{\min}(\mathbf{v})$ in the finite-dimensional case:

$$U_j^{\min}(\mathbf{v}) = \text{range}(M_j), \quad \text{where } M_j := \mathcal{M}_j(\mathbf{v}) \text{ (matricisation).}$$

The characterisation in the general case needs some notation.

V_j' dual space of V_j . Consider $\varphi^{[j]} := \bigotimes_{k \neq j} \varphi^{(k)}$ with $\varphi^{(k)} \in V_k'$. $\varphi^{[j]}$ can be regarded as a map from $\mathbf{V} = \bigotimes_{k=1}^d V_k$ onto V_j via

$$\varphi^{[j]} \left(\bigotimes_{k=1}^d v^{(k)} \right) = \left(\prod_{k \neq j} \varphi^{(k)}(v^{(k)}) \right) v^{(j)}.$$

If V_j is a normed space, V_j^* denotes the continuous dual space ($V_j^* \subset V_j'$).

Characterisations:

$$U_j^{\min}(\mathbf{v}) = \left\{ \varphi^{[j]}(\mathbf{v}) : \varphi^{[j]} \in {}_a \bigotimes_{k \neq j} V'_k \right\},$$

$$U_j^{\min}(\mathbf{v}) = \left\{ \varphi(\mathbf{v}) : \varphi \in \left({}_a \bigotimes_{k \neq j} V_k \right)' \right\},$$

although ${}_a \bigotimes_{k \neq j} V'_k$ is strictly smaller than $\left({}_a \bigotimes_{k \neq j} V_k \right)'$ in the general infinite-dimensional case.

If V_k and/or ${}_a \bigotimes_{k \neq j} V_k$ are normed spaces, even

$$U_j^{\min}(\mathbf{v}) = \left\{ \varphi^{[j]}(\mathbf{v}) : \varphi^{[j]} \in {}_a \bigotimes_{k \neq j} V_k^* \right\},$$

$$U_j^{\min}(\mathbf{v}) = \left\{ \varphi(\mathbf{v}) : \varphi \in \left({}_a \bigotimes_{k \neq j} V_k \right)^* \right\}$$

holds.

8.2 Topological Tensor Space

$(V_j, \|\cdot\|_j)$ are Banach spaces. The topological tensor space $\mathbf{V} := \|\cdot\| \otimes_{j=1}^d V_j$ is the **completion of the algebraic tensor space** ${}_a \otimes_{j=1}^d V_j$ w.r.t. a norm $\|\cdot\|$.

A necessary condition for reasonable topological tensor spaces is the **continuity of the tensor product**, i.e.,

$$\left\| \bigotimes_{j=1}^d v^{(j)} \right\| \leq C \prod_{j=1}^d \|v^{(j)}\|_j$$

for some $C < \infty$ and all $v^{(j)} \in V_j$.

DEFINITION: $\|\cdot\|$ is called a **crossnorm** if

$$\left\| \bigotimes_{j=1}^d v^{(j)} \right\| = \prod_{j=1}^d \|v^{(j)}\|_j.$$

REMARK: There are different crossnorms $\|\cdot\|$ for the same $\|\cdot\|_j$!

Reasonable Crossnorms

$\|\cdot\|_j^*$: dual norm corresponding to $\|\cdot\|_j$, i.e. $\|\varphi\|_j^* = \max\{|\varphi(v)| / \|v\|_j : 0 \neq v \in V_j\}$.

DEFINITION: $\|\cdot\|$ is called a **reasonable crossnorm** if

$$\left\| \bigotimes_{j=1}^d v^{(j)} \right\| = \prod_{j=1}^d \|v^{(j)}\|_j \quad \text{for } v^{(j)} \in V_j \quad \text{and}$$

$$\left\| \bigotimes_{j=1}^d \varphi^{(j)} \right\|^* = \prod_{j=1}^d \|\varphi^{(j)}\|_j^* \quad \text{for } \varphi^{(j)} \in V_j^*.$$

There are two extreme reasonable crossnorm. The strongest is the projective norm

$$\|\mathbf{v}\|_{\wedge} := \inf \left\{ \sum_{i=1}^m \prod_{j=1}^d \|v_i^{(j)}\|_j : \mathbf{v} = \sum_{i=1}^m \bigotimes_{j=1}^d v_i^{(j)} \right\}$$

The weakest is

DEFINITION. For $\mathbf{v} \in \mathbf{V} = a \otimes_{j=1}^d V_j$ define $\|\cdot\|_{\mathbf{V}}$ by

$$\|\mathbf{v}\|_{\mathbf{V}} := \sup \left\{ \frac{\left| \left(\varphi^{(1)} \otimes \varphi^{(2)} \otimes \dots \otimes \varphi^{(d)} \right) (\mathbf{v}) \right|}{\|\varphi^{(1)}\|_1^* \|\varphi^{(2)}\|_2^* \dots \|\varphi^{(d)}\|_d^*} : 0 \neq \varphi^{(j)} \in V_j^*, 1 \leq j \leq d \right\}.$$

(**injective norm** [Grothendieck 1953]).

THEOREM. A norm $\|\cdot\|$ on $a \otimes_{j=1}^d V_j$, for which

$$\otimes_{j=1}^d : V_1 \times \dots \times V_d \rightarrow a \otimes_{j=1}^d V_j \text{ and}$$

$$\otimes_{j=1}^d : V_1^* \times \dots \times V_d^* \rightarrow a \otimes_{j=1}^d V_j^*$$

are continuous, cannot be weaker than $\|\cdot\|_{\mathbf{V}}$, i.e.,

$$\|\cdot\| \gtrsim \|\cdot\|_{\mathbf{V}}. \quad (\text{norm})$$

We recall the definition of $\varphi^{[j]} := \bigotimes_{k \neq j} \varphi^{(k)}$ ($\varphi^{(k)} \in V'_k$) by

$$\varphi^{[j]} \left(\bigotimes_{k=1}^d v^{(k)} \right) = \left(\prod_{k \neq j} \varphi^{(k)}(v^{(k)}) \right) v^{(j)}.$$

LEMMA. $\varphi \in a \bigotimes_{k \in \{1, \dots, d\} \setminus \{j\}} V_j^*$ is continuous, i.e., $\varphi \in \mathcal{L} \left(\vee \bigotimes_{k=1}^d V_k, V_j \right)$.

Its norm is

$$\|\varphi\|_{V_j \leftarrow \vee \bigotimes_{k=1}^d V_k} = \prod_{k \in \{1, \dots, d\} \setminus \{j\}} \|v_k^*\|_k^*.$$

Consequence: $\varphi \in a \bigotimes_{k \in \{1, \dots, d\} \setminus \{j\}} V_j^*$ is well defined for topological tensors $\mathbf{v} \in \vee \bigotimes_{k=1}^d V_k$. The same conclusion holds for stronger norms than $\|\cdot\|_{\vee}$, in particular for all *reasonable crossnorms*.

Assume $\|\cdot\| \gtrsim \|\cdot\|_{\mathbf{v}}$.

MAIN THEOREM. For $\mathbf{v}_n \in \bigotimes_{j=1}^d V_j$ assume $\mathbf{v}_n \rightarrow \mathbf{v} \in \|\cdot\| \bigotimes_{j=1}^d V_j$. Then

$$\dim U_j^{\min}(\mathbf{v}) \leq \liminf_{n \rightarrow \infty} \dim U_j^{\min}(\mathbf{v}_n) \quad \text{for all } 1 \leq j \leq d.$$

THEOREM. The sets $\mathcal{T}_{\mathbf{r}}$ and $\mathcal{H}_{\mathbf{r}}$ are weakly closed.

PROOF. Let $\mathbf{v}_n \in \mathcal{T}_{\mathbf{r}}$, i.e., there are subspaces $U_{j,n}$ with $\mathbf{v}_n \in \bigotimes_{j=1}^d U_{j,n}$ and $\dim U_{j,n} \leq r_j$. Note that $U_j^{\min}(\mathbf{v}_n) \subset U_{j,n}$ with $\dim U_j^{\min}(\mathbf{v}_n) \leq r_j$.

If $\mathbf{v}_n \rightarrow \mathbf{v}$, then $\dim U_{j,\min}(\mathbf{v}) \leq r_j$ and therefore $\mathbf{v} \in \mathcal{T}_{\mathbf{r}}$. Similar for $\mathcal{H}_{\mathbf{r}}$.

Application to Best Approximation

THEOREM. Let $(X, \|\cdot\|)$ be a reflexive Banach space with a weakly closed subset $\emptyset \neq M \subset X$. Then for any $x \in X$ there exists a **best approximation** $v \in M$ with

$$\|x - v\| = \inf\{\|x - w\| : w \in M\}.$$

LEMMA A. If $x_n \rightharpoonup x$, then $\|x\| \leq \liminf_{n \rightarrow \infty} \|x_n\|$.

LEMMA B. If X is a reflexive Banach space, any bounded sequence $x_n \in X$ has a subsequence x_{n_i} converging weakly to some $x \in X$.

PROOF of the Theorem. Choose $w_n \in M$ with $\|x - w_n\| \rightarrow \inf\{\|x - w\| : w \in M\}$. Since $(w_n)_{n \in \mathbb{N}}$ is a bounded sequence in X , LEMMA B ensures the existence of a subsequence $w_{n_i} \rightharpoonup v \in X$. v belongs to M because $w_{n_i} \in M$ and M is weakly closed. Since also $x - w_{n_i} \rightharpoonup x - v$, LEMMA A shows $\|x - v\| \leq \liminf \|x - w_{n_i}\| \leq \inf\{\|x - w\| : w \in M\}$.

Conclusion for $M \in \{\mathcal{T}_r, \mathcal{H}_r\}$:

COROLLARY. Let $\|\cdot\|$ satisfy $\|\cdot\| \gtrsim \|\cdot\|_V$ and let $(V, \|\cdot\|_V)$ be reflexive. Then best approximations in the formats \mathcal{T}_r and \mathcal{H}_r exist.

9 Properties of the HOSVD Projection

We recall: The Tucker and hierarchical representation may be based on the HOSVD bases $\{b_\ell^{(\alpha)} : 1 \leq \ell \leq r_\alpha\}$. The HOSVD projection is of the form

$$P = P_\alpha \otimes P_{\alpha^c} \quad \text{with } P_\alpha b_\ell^{(\alpha)} = \begin{cases} b_\ell^{(\alpha)} & \text{for } 1 \leq \ell \leq s_\alpha, \\ 0 & \text{for } s_\alpha < \ell \leq r_\alpha \end{cases}$$

Let

$$\mathbf{u}_{\text{HOSVD}} = P\mathbf{v}.$$

LEMMA. Let $\phi_j \mathbf{v} = 0$ for some $\phi_j = id \otimes \dots \otimes \varphi_j \otimes id \otimes \dots \otimes id$, $\varphi_j \in V_j'$. Then also $\phi_j \mathbf{u}_{\text{HOSVD}} = 0$.

LEMMA. If $\mathbf{v} \in \mathbf{V}$ belongs to the domain of ϕ_j , then also $\mathbf{u}_{\text{HOSVD}}$ belongs to the domain and satisfies

$$\|\phi_j \mathbf{u}_{\text{HOSVD}}\| \leq \|\phi_j \mathbf{v}\|.$$

Application: $\|\partial^k \mathbf{u}_{\text{HOSVD}} / \partial x_j^k\|_{L^2} \leq \|\partial^k \mathbf{v} / \partial x_j^k\|_{L^2}$.

L^∞ Estimates

Problem:

- HOSVD projection uses the underlying Hilbert norm (L^2)
- Pointwise evaluations require the maximum norm (L^∞)

Gagliardo-Nirenberg inequality:

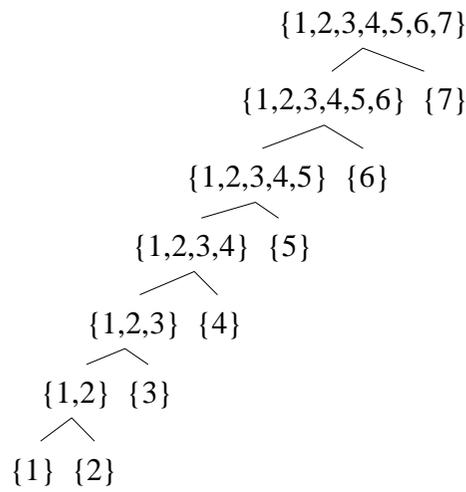
$$\|\varphi\|_\infty \leq c_m^\Omega |\varphi|_m^{\frac{d}{2m}} \|\varphi\|_{L^2}^{1 - \frac{d}{2m}}, \quad \text{where}$$
$$|\varphi|_m := \left(\int_\Omega \sum_{j=1}^d \left| \frac{\partial^m \varphi}{\partial x_j^m} \right|^2 dx \right)^{1/2}.$$

For $\Omega = \mathbb{R}^d$ we have

$$\lim_{m \rightarrow \infty} c_m^\Omega = \pi^{-d/2}.$$

10 Graph-Based Formats

10.1 Matrix-Product (TT) Format



A particular binary tree is $\{1\} \{2\}$. It leads to the TT format (Oseledets–Tyrttyshnikov 2005) and coincides with the description of the matrix product states (Vidal 2003, Verstraete–Cirac 2006) used in physics:

Each component $\mathbf{v}[i_1, \dots, i_d]$ of $\mathbf{v} \in \mathbf{V} = \bigotimes_{j=1}^d \mathbb{K}^{n_j}$ is expressed by

$$\mathbf{v}[i_1 i_2 \cdots i_d] = M^{(1)}[i_1] \cdot M^{(2)}[i_2] \cdot \dots \cdot M^{(d-1)}[i_{d-1}] \cdot M^{(d)}[i_d] \in \mathbb{K},$$

where $M^{(j)}[i]$ are matrices of size $r_{j-1} \times r_j$ with $r_0 = r_d = 1$.

To avoid the special roles of the vectors $M^{(1)}[i_1]$, $M^{(d)}[i_d]$ and to describe periodic situations, the **Cyclic Matrix-Product format** $\mathcal{C}(d, (r_j), (n_j))$, $n_j = \dim V_j$, is used in physics:

$$\begin{aligned} \mathbf{v}[i_1 i_2 \cdots i_d] &= \text{trace}\{M^{(1)}[i_1] \cdot M^{(2)}[i_2] \cdots \cdots M^{(d-1)}[i_{d-1}] \cdot M^{(d)}[i_d]\} \\ &= \sum_{k_1=1}^{r_1} \cdots \sum_{k_d=1}^{r_d} M_{k_d k_1}^{(1)}[i_1] \cdot M_{k_1 k_2}^{(2)}[i_2] \cdots \cdots M^{(d-1)}[i_{d-1}] \cdot M_{k_{d-1} k_d}^{(d)}[i_d]. \end{aligned}$$

Tensor Network: tensor representations based on general graphs.

THEOREM (Landsberg–Qi–Ye 2012) Formats based on a graph \neq tree are in general not closed.

10.2 Intermezzo: Algebra Structure Tensors

V algebra, i.e. vector space with additional operation \circ , $\{b_k\}$ basis of V .
The operation is completely described by the coefficients s_{ijk} in

$$b_i \circ b_j = \sum_k s_{ijk} b_k.$$

Let $b_i^* \in V'$ the dual element with $\langle \sum_k \alpha_k b_k, b_i^* \rangle = \alpha_i$. Then

$$\mathbf{s} := \sum_{i,j,k} s_{ijk} b_i^* \otimes b_j^* \otimes b_k \in V' \otimes V' \otimes V$$

is the *structure tensor* of the algebra.

Remark. For $v, w \in V$ we have $v \circ w = (v \otimes w \otimes id) \mathbf{s}$.

Proof: Let $v = \sum_i v_i b_i$ and $w = \sum_j w_j b_j$. Then

$$\begin{aligned} (v \otimes w \otimes id) \mathbf{s} &= \sum_{i,j,k} s_{ijk} \langle v, b_i^* \rangle \langle w, b_j^* \rangle b_k = \sum_{i,j,k} s_{ijk} v_i w_j b_k = \sum_{i,j} v_i w_j \sum_k s_{ijk} b_k \\ &= \sum_{i,j} v_i w_j b_i \circ b_j = \left(\sum_i v_i b_i \right) \circ \left(\sum_j w_j b_j \right) = v \circ w. \end{aligned}$$

Matrix Multiplication

Consider $V = \mathbb{K}^{2 \times 2}$, $\circ = *$ is the matrix multiplication.

The basis of V is $\{E_{pq} : 1 \leq p, q \leq 2\}$, where $E_{pq}[i, j] = \begin{cases} 1 & \text{for } (i, j) = (p, q) \\ 0 & \text{otherwise.} \end{cases}$

LEMMA. The structure tensor of the matrix multiplication is

$$\mathbf{m} := \sum_{i_1=1}^2 \sum_{i_2=1}^2 \sum_{i_3=1}^2 E_{i_1, i_2}^* \otimes E_{i_2, i_3}^* \otimes E_{i_1, i_3} \in V' \otimes V' \otimes V.$$

Proof. Let $A, B \in \mathbb{K}^{2 \times 2}$ and $C := AB$. Then

$$(A \otimes B \otimes id)\mathbf{m} = \sum_{i_1, i_2, i_3=1}^2 A_{i_1, i_2} B_{i_2, i_3} E_{i_1, i_3} = \sum_{i_1, i_3=1}^2 C_{i_1, i_3} E_{i_1, i_3} = C.$$

THEOREM: $\text{rank}(\mathbf{m}) = \underline{\text{rank}}(\mathbf{m}) = 7$.

Strassen, 1969: $\text{rank}(\mathbf{m}) \leq 7$; Winograd, 1971: $\text{rank}(\mathbf{m}) = 7$;

Landsberg, 2012: $\underline{\text{rank}}(\mathbf{m}) = 7$.

10.3 Cyclic Matrix-Product Format

We recall the Cyclic Matrix-Product Format $\mathcal{C}(d, (r_j), (n_j))$

$$\begin{aligned} \mathbf{v}[i_1 i_2 \cdots i_d] &= \text{trace}\{M^{(1)}[i_1] \cdot M^{(2)}[i_2] \cdot \cdots \cdot M^{(d-1)}[i_{d-1}] \cdot M^{(d)}[i_d]\} \\ &= \sum_{k_1=1}^{r_1} \cdots \sum_{k_d=1}^{r_d} M_{k_d k_1}^{(1)}[i_1] \cdot M_{k_1 k_2}^{(2)}[i_2] \cdot \cdots \cdot M^{(d-1)}[i_{d-1}] \cdot M_{k_{d-1} k_d}^{(d)}[i_d]. \end{aligned}$$

A subcase is the **site-independent format** Matrix-Product Format $\mathcal{C}_{\text{ind}}(d, r, n)$ with

$$\begin{aligned} M^{(j)}[i] &= M[i] \\ r_j &= r, \\ V_j &= V \quad \text{for all } j, \\ n &= \dim V. \end{aligned}$$

THEOREM (Landsberg–Qi–Ye 2012) Formats based on a graph \neq tree are in general not closed.

10.4 Result for $d = 3$, $V = \otimes^3 \mathbb{K}^{2 \times 2}$, $r_1 = r_2 = r_3 = 2$ by Harris–Michalek–Sertöz 2018

Let

$$\mathbf{m} := \sum_{k_1, k_2, k_3=1}^2 E_{k_3, k_1} \otimes E_{k_1 k_2} \otimes E_{k_2, k_3} \in \bigotimes_{j=1}^3 \mathbb{K}^{2 \times 2}.$$

$\{E_{pq} : 1 \leq p, q \leq 2\}$ is the canonical basis of $\mathbb{K}^{2 \times 2}$.

LEMMA. Let $V = \otimes_{j=1}^3 \mathbb{K}^{2 \times 2}$. The set $\mathcal{C}(d = 3, (r_j = 2), (n_j = 4))$ consists of all

$$\mathbf{v} = \Phi(\mathbf{m}) \quad \text{with} \quad \Phi = \bigotimes_{j=1}^3 \phi^{(j)} \quad \text{and} \quad \phi^{(j)} \in L(\mathbb{K}^{2 \times 2}, \mathbb{K}^{2 \times 2}).$$

REMARK. a) \mathbf{m} is equivalent to the Strassen tensor of the matrix multiplication.

b) If all $\phi^{(j)}$ are bijective, $\mathbf{v} = \Phi(\mathbf{m})$ implies that $\text{rank}(\mathbf{v}) = 7$.

We consider the *site-independent* case $M^{(j)}[i] = M[i]$ for all $1 \leq j \leq d := 3$.

Define $\psi \in L(\mathbb{K}^{2 \times 2}, \mathbb{K}^{2 \times 2})$ by $\psi(E_{12}) = E_{12} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ and $\psi(E_{pq}) = 0$ for $(p, q) \neq (1, 2)$ and

$$\mathbf{v}(t) = \left(\otimes^3(\psi + t \cdot id) \right) (\mathbf{m}) = \mathbf{v}_0 + t \cdot \mathbf{v}_1 + t^2 \cdot \mathbf{v}_2 + t^3 \cdot \mathbf{v}_3 \in \mathcal{C}_{\text{ind}}(3, 2, 4)$$

with

$$\begin{aligned} \mathbf{v}_0 &= (\otimes^3 \psi)(\mathbf{m}), & \mathbf{v}_1 &= [\psi \otimes \psi \otimes id + \psi \otimes id \otimes \psi + id \otimes \psi \otimes \psi](\mathbf{m}), \\ \mathbf{v}_2 &= [id \otimes id \otimes \psi + id \otimes \psi \otimes id + \psi \otimes id \otimes id](\mathbf{m}), & \mathbf{v}_3 &= \mathbf{m}. \end{aligned}$$

$\Rightarrow \mathbf{v}_0 = \mathbf{v}_1 = 0$ and

$$\begin{aligned} \mathbf{v}_2 &= E_{21} \otimes E_{11} \otimes E_{12} + E_{22} \otimes E_{21} \otimes E_{12} + E_{11} \otimes E_{12} \otimes E_{21} \\ &\quad + E_{21} \otimes E_{12} \otimes E_{22} + E_{12} \otimes E_{21} \otimes E_{11} + E_{12} \otimes E_{22} \otimes E_{21}, \end{aligned}$$

$\Rightarrow \text{rank}(\mathbf{v}_2) \leq 6$. The following limit exists:

$$\mathbf{v}_2 = \lim_{t \rightarrow 0} t^{-2} \mathbf{v}(t) \in \text{closure}(\mathcal{C}_{\text{ind}}(3, 2, 4)).$$

The non-closedness of $\mathcal{C}_{\text{ind}}(3, 2, 4)$ will follow from $\mathbf{v}_2 \notin \mathcal{C}_{\text{ind}}(3, 2, 4)$.

For an indirect proof **assume** $\mathbf{v}_2 \in \mathcal{C}_{\text{ind}}(3, 2, 4)$. The Lemma implies that there is some $\phi \in L(\mathbb{K}^{2 \times 2}, \mathbb{K}^{2 \times 2})$ with $\mathbf{v}_2 = (\otimes^3 \phi)(\mathbf{m})$.

It is easy to check that the range of the matricisation

$$\mathcal{M}_1((\otimes^3 \phi)(\mathbf{m})) = \phi \mathcal{M}_1(\mathbf{m}) (\otimes^2 \phi)^\top$$

is $\mathbb{K}^{2 \times 2}$. Therefore the map ϕ must be surjective.

Since $\phi \in L(\mathbb{K}^{2 \times 2}, \mathbb{K}^{2 \times 2})$ is surjective, it is also injective and thus bijective.

By Remark (b) $\text{rank}(\mathbf{v}_2) = \text{rank}(\mathbf{m}) = 7$ holds in contradiction to $\text{rank}(\mathbf{v}_2) \leq 6$.

This contradiction proves that $\mathbf{v}_2 \notin \mathcal{C}_{\text{ind}}(3, 2, 4)$.

Similarly $\mathbf{v}_2 \notin \mathcal{C}(3, (2, 2, 2), (4, 4, 4))$ follows (no site-independence).

10.5 Result for $V = \otimes^d \mathbb{C}^2$, $r_j = 2$

Smallest (nontrivial) dimension: $V_j = \mathbb{C}^2$,

tensor space $V = \otimes^d \mathbb{C}^2$

Site-independent cyclic format $\mathcal{C}_{\text{ind}}(d, 2, 2)$, i.e., $r = 2$

Result:

$d = 3$: $\mathcal{C}_{\text{ind}}(3, 2, 2)$ is closed (cf. Harris–Michalek–Sertöz 2018)

$d > 3$: $\mathcal{C}_{\text{ind}}(d, 2, 2)$ is not closed (cf. Tim Seynnaeve 2018)

Same for $\mathbb{K} = \mathbb{R}$

Extension to Larger Spaces

$d \geq 4$:

$\mathcal{C}_{\text{ind}}(d, r = 2, n = 2)$ not closed $\Rightarrow \mathcal{C}_{\text{ind}}(d, r = 2, n)$ not closed for all $n \geq 2$.

Missing case

$\mathcal{C}_{\text{ind}}(3, 2, 2)$ closed, $\mathcal{C}_{\text{ind}}(3, 2, 4)$ not closed

Also $\mathcal{C}_{\text{ind}}(3, 2, 3)$ is not closed (Tim Seynnaeve, technical proof).

Case of $r \geq 3$

$\mathbf{V}_{\text{cycl}} := \{\mathbf{v} \in \mathbf{V} : \pi \mathbf{v} = \mathbf{v}\}$ for $\pi : (1, 2, \dots, d) \mapsto (2, \dots, d, 1)$

Let $d > 3$, $n \geq 2$, $\mathbb{K} = \mathbb{C}$ or d odd:

a) $\mathcal{C}_{\text{ind}}(d, r, n)$ not closed for $r = 2$

b) r sufficiently large $\Rightarrow \mathcal{C}_{\text{ind}}(d, r, n) = \mathbf{V}_{\text{cycl}} \Rightarrow \mathcal{C}_{\text{ind}}(d, r, n)$ closed.

Another reason for closedness of $\mathcal{C}_{\text{ind}}(3, 2, 2)$ (Proof: Tim Seynnaeve):

$$\mathcal{C}_{\text{ind}}(3, 2, 2) = \mathbf{V}_{\text{cycl}}.$$

11 Tensorisation

$V_j = \mathbb{R}^n \Rightarrow$ storage: $rdn + (d - 1)r^3$. Now: $n \rightarrow O(\log n)$

Let the vector $y \in \mathbb{R}^n$ represent the grid values of a function in $(0, 1]$:

$$y_\mu = f\left(\frac{\mu + 1}{n}\right) \quad (0 \leq \mu \leq n - 1).$$

Choose, e.g., $n = 2^d$, and note that $\mathbb{R}^n \cong \mathbf{V} := \bigotimes_{j=1}^d \mathbb{R}^2$.

Isomorphism by binary integer representation:

$\mu = \sum_{j=1}^d \mu_j 2^{j-1}$ with $\mu_j \in \{0, 1\}$, i.e.,

$$y_\mu = \mathbf{v}[\mu_1, \mu_2, \dots, \mu_{d-1}, \mu_d].$$

Algebraic Function Compression (black-box procedure)

- 1) Tensorisation: $y \in \mathbb{R}^n \mapsto \mathbf{v} \in \mathbf{V}$ (storage size: $n = 2^d$)
- 2) Apply the *tensor truncation*: $\mathbf{v} \mapsto \mathbf{v}_\varepsilon$
- 3) Observation: often the data size decreases from $n = 2^d$ to $O(d) = O(\log n)$.

EXAMPLE

$y \in \mathbb{C}^n$ with $y_\mu = \zeta^\mu$ leads to an *elementary tensor* $\mathbf{v} \in \mathbf{V}$, i.e.,

$$\mathbf{v} = \bigotimes_{j=1}^d v^{(j)} \quad \text{with } v^{(j)} = \begin{bmatrix} 1 \\ \zeta^{2^{j-1}} \end{bmatrix} \in \mathbb{C}^2.$$

Storage size = $2d = 2 \log_2 n$.

Consequence:

All functions $f \in C((0, 1])$, which can be well-approximated by r *trigonometric terms* or *exponential sums* with r terms (even with complex coefficients \rightarrow Bessel functions) can be approximated by a tensor representation with data size

$$2dr = O(r \log n).$$

Example:

$f(x) = 1/(x + \delta) \in C((0, 1])$, $\delta \geq 0$, can be well-approximated by exponential sums (cf. Braess-H.):

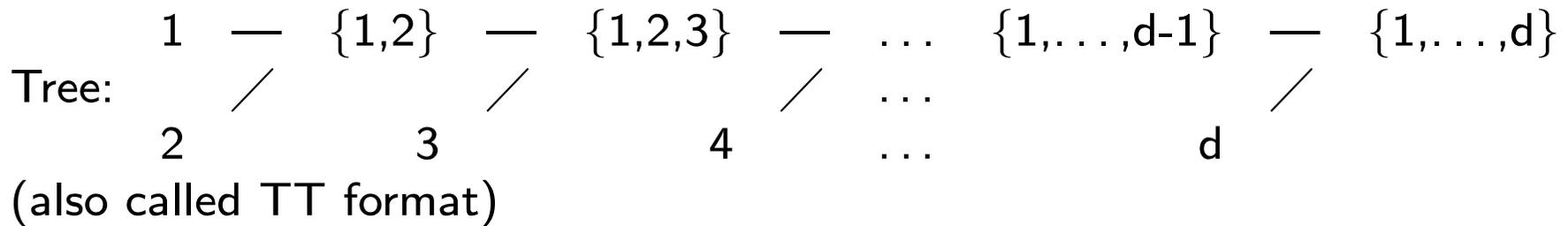
$$f(x) \approx \sum_{\nu=1}^r a_{\nu} \exp(-b_{\nu}x) \quad (a_{\nu}, b_{\nu} > 0)$$

error: $O(n \exp(-2^{1/2} \pi r^{1/2}))$ if $\delta = 0$,
 $O(\exp(-cr))$ if $\delta = O(1)$.

Storage size:

$$2dr = 2r \log_2 n = O(\log^2(\varepsilon) \log(n))$$

Hierarchical Format, Matricisation



Consider the tensorisation $\mathbf{v} \in \bigotimes_{j=1}^d \mathbb{R}^2$ of the vector $y = (y_0, \dots, y_{n-1}) \in \mathbb{R}^n$.
 The matricisation for $\alpha = \{1, \dots, j\}$ ($1 \leq j \leq d-1$) yields

$$\mathcal{M}_\alpha(\mathbf{v}) = \begin{bmatrix} y_0 & y_m & \cdots & y_{n-m} \\ y_1 & y_{m+1} & \cdots & y_{n-m+1} \\ \vdots & \vdots & & \vdots \\ y_{m-1} & y_{2m-1} & \cdots & y_{n-1} \end{bmatrix} \text{ with } m := 2^j.$$

Recall: $\text{rank}_\alpha(\mathbf{v}) = \dim \mathcal{M}_\alpha(\mathbf{v})$.

p-Methods

$$f(x) \approx \tilde{f}(x) = \sum_{k=1}^r a_k e^{2\pi i(k-1)x} \text{ trigonometric approximation}$$

\Rightarrow tensorisation, storage $2dr = 2r \log_2 n$, error $\leq \|f - \tilde{f}\|$

Similar for $\tilde{f}(x) = \sum_{k=1}^r a_k \sin(2\pi ik)$ etc.

Polynomials:

$f(x) \approx P(x)$, P polynomial of degree $\leq p$

An r -term representation $\sum_{i=1}^r \bigotimes_{j=1}^d v_i^{(j)}$ does not work well.

Instead, the hierarchical format (in particular, the TT format) is used.

Conclusion for polynomial p-methods

If $\mathbf{f} \approx \mathbf{P}$ with a polynomial \mathbf{P} of degree $\leq p$ (\Rightarrow data size $p + 1$), then the tensorised grid function \mathbf{f} can be approximated by a tensor $\tilde{\mathbf{f}}$ such that the TT ranks are bounded by $\rho_j \leq p + 1$:

$$\|\mathbf{f} - \tilde{\mathbf{f}}\|_2 \leq \|\mathbf{f} - \mathbf{P}\|_2$$

The data size is bounded by

$$\leq 2d(p + 1)^2 .$$

hp Method

Let f be an asymptotically smooth function in $(0, 1]$ with possible singularity at $x = 0$, e.g., $f(x) = x^x$.

Use the (best) piecewise polynomial approximation \tilde{f} (by degree p) in all intervals

$$\left[0, \frac{1}{n}\right], \left[\frac{1}{n}, \frac{2}{n}\right], \left[\frac{2}{n}, \frac{4}{n}\right], \dots, \left[\frac{1}{4}, \frac{1}{2}\right], \left[\frac{1}{2}, 1\right].$$

Required data size of hp method: $(p + 1) \log_2 n$.

Tensor ranks:

$$r_1 \leq \dim(\text{span}\{\tilde{f}|_{[(\mu-1)h, \mu h]} : 1 \leq \mu \leq n\}) \leq p + 1,$$

$$r_2 \leq \dim(\text{span}\{\tilde{f}|_{[(\mu-1)2h, \mu 2h]} : 1 \leq \mu \leq \frac{n}{2}\}) \leq p + 2,$$

$$r_3 \leq \dim(\text{span}\{\tilde{f}|_{[(\mu-1)4h, \mu 4h]} : 1 \leq \mu \leq \frac{n}{4}\}) \leq p + 2,$$

⋮

Hence, the data size of the tensorisation of \tilde{f} is bounded by

$$d(p + 2)^2 = (p + 2)^2 \log_2 n.$$

THEOREM (Grasedyck 2010) f asymptotically smooth with m point singularities. Then the data size of v_ε corresponding exactly to a piecewise polynomial approximation is characterised by

$$r = O(1) + \log_2 \frac{1}{\varepsilon} + 2m.$$