Manifolds and tangent spaces of TT and HT tensors

R. Schneider (TUB Matheon)

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Noteable special case of HT:

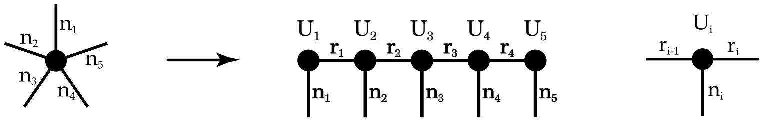
TT format (Oseledets & Tyrtyshnikov, 2009)
(matrix product states (MPS), Vidal 2003, Schöllwock et al.)

TT tensor U can be written as matrix product form

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

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

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



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

Setting - Tensors

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

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

The function $U \in \mathcal{H}$ will be called an order d-tensor.
For notational simplicity, we often consider $n_i = n$. Here
$x_1, \ldots, x_d \in \{1, \ldots, n\}$ will be called variables or indices.

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

Or in index (vectorial) notation

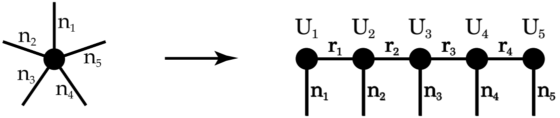
$$\mathbf{U} = \left(U_{k_1,\ldots,k_d}\right)_{k_i=0,1\leq i\leq d}^{n_i}$$

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

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

II.

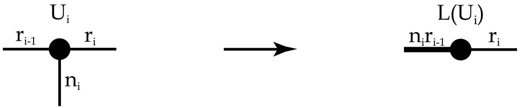
Existence and uniqueness results



Definitions: Left and right unfoldings

- Left unfolding of comp. functions $\mathbf{U}_i : x_i \to \mathbf{U}_i(x_i) \in \mathbb{R}^{r_{i-1} \times r_i}$: Matrix

$$\mathbf{L}\big(\mathbf{U}_i(x_i)\big) := U^{k_i}_{x_i, k_{i-1}} \in \mathbb{R}^{(r_{i-1} n_i) \times r_i}$$



- Left rank of $\mathbf{U}_i$ is rank $\mathbf{L}\big(\mathbf{U}(x_i)\big)$,
- $\mathbf{U}_i$ is left orthogonal if $\mathbf{L}\big(\mathbf{U}_i(x_i)\big) \in \mathcal{O}(\mathbb{R}^{(n_i r_{i-1}) \times r_i})$
- Right unfolding, right orthogonality, right rank: Via

$$\mathbf{R}\big(\mathbf{U}(x_i)\big) := U^{x_i, k_i}_{k_{i-1}}.$$

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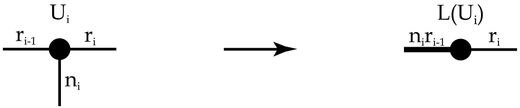

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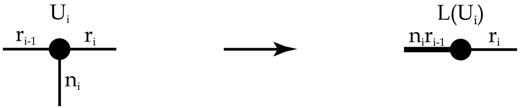

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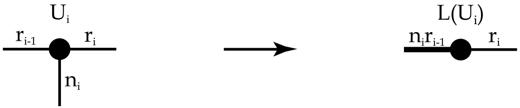

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Definitions: TT rank, separation rank

$\mathbf{U}_i(x_i) : \{1, \ldots, n_i\} \to \mathbb{R}^{r_{i-1} \times r_i}$ satisfies full rank condition iff

$$\boxed{\text{rank}\, \mathbf{L}\big(\mathbf{U}_i(x_i)\big) \;=\; r_i \;=\; \text{rank}\, \mathbf{R}\big(\mathbf{U}_{i+1}(x_{i+1})\big).}$$

If all component functions $\mathbf{U}_i(x_i)$ of a TT decomposition

$$U(\mathbf{x}) \;=\; \mathbf{U}_1(x_1)\mathbf{U}_2(x_2) \cdot \ldots \cdot \mathbf{U}_{d-1}(x_{d-1})\mathbf{U}_d(x_d)$$

satisfy the full rank condition, the above decomposition is

a decomposition of TT rank $\underline{r} = (r_1, \ldots, r_{d-1})$.

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i-th seperation rank s_i of U:

$$\text{Rank of } \mathbf{A}_i = U_{x_1,\ldots,x_i}^{x_{i+1},\ldots,d}.$$

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Existence and “uniqueness” of TT decompositions

Theorem (Holtz, R., Schneider, 2010)

- *There is exactly one rank vector* $\underline{r} = (r_1, \ldots, r_{d-1})$ *such that* U *admits for a TT decomposition of full rank* $\underline{r}$.
  (i.e., s.t. component functions satisfy full rank condition).

  For other TT decompositions, $r_i' \geq r_i$ *for all* $i = 1, \ldots, d-1$

- $\boxed{r_i = s_i}$ *(separation ranks) for* $i = 1, \ldots, d-1$

- *Component functions can be chosen left-orthonormal for* $i = 1, \ldots, d-1$*; then*

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

iff *for some* $\mathbf{Q}_i \in \mathcal{O}(\mathbb{R}^{r_i \times r_i})$,

$$\mathbf{U}_1(x_1)\mathbf{Q}_1 = \mathbf{V}_1(x_1), \quad \mathbf{Q}_{d-1}^T \mathbf{U}_d(x_d) = \mathbf{V}_d(x_d),$$

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Principle bundle

Consider the (linear) parameter space

$$\times_{i=1}^{d} X_i \quad , \quad X_i := \mathbb{R}^{r_{i-1} \times n_i \times r_i}$$

We define (Lie) group action (cf. *Uschmajev*)

$$G_i U_i := \mathbf{G}_{i-1}^{-1} \mathbf{U}_i(x_i) \mathbf{G}_i \ , \ i = 1, \ldots, d-1, \quad U_i \in X_i \ .$$

with the invertible matrices $G_i \in GL(R^{r_i})$, forming a Lie group.
And define the Lie group

$$\underline{G} \in \mathcal{G}_{\underline{r}} := \times_{i=1}^{d-1} GL(R^{r_i}) \quad , \ \mathcal{G}_{\underline{r}} U := (G_i U_i)_{i=1}^{d}$$

this but induces an equivalence relation

$$\underline{U} \sim \underline{V} \quad \Leftrightarrow \underline{U} = \underline{G}\underline{V} \ , \underline{G} \in \mathcal{G}_{\underline{r}}$$

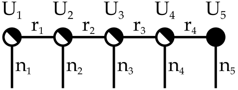
and equivalence classes. This does not only removes the redundancy, but also defines a manifold *Lubich & Koch, Rohwedder & S. , Uschmajev &Vandereycken, Arnold & Jahnke*

$$\boxed{\mathcal{M}_{\underline{r}} \eqsim \left(\times_{i=1}^{d} X_i \right) / \mathcal{G}_{\underline{r}}}$$

III.

The manifold of tensors of fixed TT rank *r*

$$\mathbb{T} := \mathbb{T}_{\underline{r}} := \{U \in \mathbb{R}^{n_1 \times \ldots \times n_d} \text{ tensor of TT rank } \underline{r}\}.$$



Unique representation of the tangent space of $\mathbb{T}$

Theorem (Holtz, R. Schneider, 2010)

For all $U \in \mathbb{T}$, and for

$$\delta U \in \mathcal{T}_U \mathbb{T} \simeq \Big\{ \gamma'(t)|_{t=0} \mid \gamma \in C^1(]-\delta, \delta[, \mathbb{T}), \quad \gamma(t) = \mathbf{U}_1(x_1, t) \cdot \ldots \cdot \mathbf{U}_d(x_d, t), \;\; \gamma(0) = U(\underline{x}) \Big\}$$

there is a unique vector $(\mathbf{W}_1 \ldots, \mathbf{W}_d)$ of component functions $\mathbf{W}_i(\cdot) : \mathcal{I}_i \to \mathbb{R}^{r_{i-1} \times r_i}$, such that

$$\boxed{\delta U = \delta U_1 + \ldots + \delta U_d}$$

with

$$\boxed{\delta U_i := \mathbf{U}_1(x_1) \ldots \mathbf{U}_{i-1}(x_{i-1}) \mathbf{W}_i(x_i) \mathbf{U}_{i+1}(x_{i+1}) \ldots \mathbf{U}_d(x_d),}$$

and s.t. $\mathbf{W}_i(\cdot)$ fulfil the (left-orthogonality) gauge conditions

$$\boxed{\mathbf{L}(\mathbf{U}_i)^T \mathbf{L}(\mathbf{W}_i) = \mathbf{0} \in \mathbb{R}^{r_i \times r_i} \quad \text{for } i = 1, .., d-1.}$$

Sketch of proof

- Existence:

$$\delta U \simeq \mathbf{U}_1'(x_1,0)\mathbf{U}_2(x_2)\cdot .. \cdot \mathbf{U}_d(x_d) + \mathbf{U}_1(x_1)\mathbf{U}_2'(x_2,0)\cdot .. \cdot \mathbf{U}_d(x_d) + \dots + \mathbf{U}_1(x_1)\cdot .. \cdot \mathbf{U}_{d-1}(x_{d-1})\mathbf{U}_d'(x_d,0).$$

Left orthogonal decomposition: there ex. unique Λ_1 s.t.

$$\mathbf{U}'(x_1,0) = \mathbf{U}_1(x_1)\Lambda_1 + \mathbf{W}_1(x_1),$$

iterate.

- Uniqueness: (Idea from Lubich et al., Tucker format)
  - Testing δU with

    $$V_i(x) := \mathbf{U}_1(x_1)\cdot .. \cdot \mathbf{U}_{i-1}(x_{i-1})\mathbf{V}_i(x_i)\mathbf{U}_{i+1}(x_{i+1}) .. \cdot \mathbf{U}_d(x_d),$$

    for $i = 1, .., d$, gauge condition (in other inner product) gives upper block-Δ-system with SPD matrices.
  - $\mathbf{L}(\mathbf{W}_i)$, $i = d, d-1, .., 1$ can uniquely be computed recursively.

Parametrization of $\mathcal{T}_U\mathbb{T}$

- C_i spaces of component functions $\mathbf{U}_i$, $(i = 1, .., d)$
- Left-orthonormal spaces of $\mathbf{U}_i$:

$$U_i^\ell := \{\mathbf{W}_i(x_i) \in C_i,\ \ \mathbf{L}(\mathbf{U}_i)^T\mathbf{L}(\mathbf{W}_i) = \mathbf{0}\}.$$

- Parameter space $X := U_1^\ell \times \ldots \times U_{d-1}^\ell \times C_d$.

Corollary (Holtz, R., Schneider, 2010)

The mapping $\tau : X \to \hat{\mathcal{T}}_U\mathbb{T}$,

$$\tau(\mathbf{W}_1, \ldots, \mathbf{W}_d) \ = \ \sum_{i=1}^{d} \mathbf{U}_1 \cdot \ldots \cdot \mathbf{U}_{i-1}\mathbf{W}_i\mathbf{U}_{i+1} \cdot \ldots \cdot \mathbf{U}_d$$

is a linear bijection between X *and* $\mathcal{T}_U\mathbb{T}$*. In particular,*

$$dim\ \mathbb{T} \ = \ \sum_{i=1}^{d} r_{i-1}n_ir_i - \sum_{i=1}^{d-1} r_i^2.$$

Local parametrization for $\mathbb{T}$

Theorem (Holtz, R., Schneider, 2010)

Let $U \in \mathbb{T}$, $\Psi : X \to \mathcal{H}$ defined by

$$\boxed{\Psi(\mathbf{W}_1, \ldots, \mathbf{W}_d) \;=\; (\mathbf{U}_1 + \mathbf{W}_1)(x_1) \cdot .. \cdot (\mathbf{U}_d + \mathbf{W}_d)(x_d).}$$

- *There exists open $N_\delta(0) \subseteq \mathbb{R}^{\dim X}$ such that*

$$\Psi|_{N_\delta} : \quad N_\delta(0) \mapsto \Psi(N_\delta(0)) \overset{open}{\subseteq} \mathbb{T}$$

is an embedding (i.e. an immersion that is a homeomorphism onto its image),
that is, $N_U \cap \mathbb{T}$ is a regular submanifold of $\mathcal{H}$.

- *There exists $N_\delta \subset \mathcal{H}$ open, a constraint function*
$g = g_U : N_\delta \to \mathbb{R}^c$, $c = \sum_{i=1}^{d-1} r_i^2$, such that

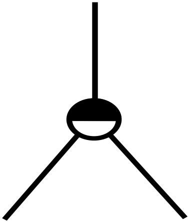
$$N_\delta \cap \mathbb{T} \;=\; \{U \in \mathbb{R}^{n^d} : g(U) = 0\} \;=\; \psi(N_\delta(0))$$

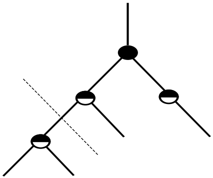
Proof: Inv. mapping theorem for manifolds, tang. space par. τ

Hierarchical Tucker format: recursive describtion

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

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





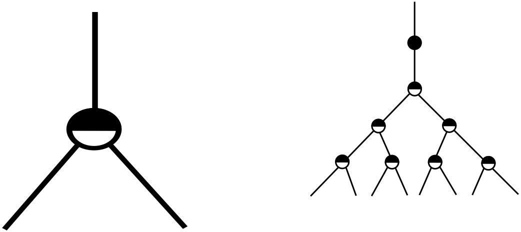
Coefficients $c_{ij}^{(\alpha,\ell)}$ form the matrices $C^{(\alpha,\ell)}$.

Final representation of $\mathbf{v}$ is

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

Recursive describtion: orthonormal basis

$\{\mathbf{b}_i^{(\alpha)} : 1 \leq i \leq r_\alpha\}$ 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 $\left\{C^{(\alpha,\ell)} : 1 \leq \ell \leq r_\alpha\right\}$ are orthonormal (w.r.t. the Frobenius scalar product).

Tangent tensors. recursive describtion

Let $\mathbf{v}(t)$ be a differentiable function. We characterise $\dot{\mathbf{v}}(t)$ at $t = 0$ and abbreviate $\dot{\mathbf{v}} := \dot{\mathbf{v}}(0)$, $(\mathrm{r}_D = 1)$,

$$\dot{\mathbf{v}} = \dot{c}_1^{(D)}\mathbf{b}_1^{(D)} + c_1^{(D)}\dot{\mathbf{b}}_1^{(D)}.$$

$$\dot{\mathbf{b}}_\ell^{(\alpha)} = \sum_{i=1}^{r_{\alpha_1}}\sum_{j=1}^{r_{\alpha_2}} \dot{c}_{ij}^{(\alpha,\ell)}\,\mathbf{b}_i^{(\alpha_1)}\otimes\mathbf{b}_j^{(\alpha_2)} + \sum_{i=1}^{r_{\alpha_1}}\sum_{j=1}^{r_{\alpha_2}} c_{ij}^{(\alpha,\ell)}\,\dot{\mathbf{b}}_i^{(\alpha_1)}\otimes\mathbf{b}_j^{(\alpha_2)} + \sum_{i=1}^{r_{\alpha_1}}\sum_{j=1}^{r_{\alpha_2}} c_{ij}^{(\alpha,\ell)}\,\mathbf{b}_i^{(\alpha_1)}\otimes\dot{\mathbf{b}}_j^{(\alpha_2)}$$

$\dot{\mathbf{v}}$ is recursively determined by

$$\dot{c}_1^{(D)}\ ,\ c_1^{(D)}\ ,\ \dot{c}_{ij}^{(\alpha,\ell)}\ ,\ c_{ij}^{(\alpha,\ell)}\ \text{ and }\ \dot{b}_i^{(j)}\ ,\ b_i^{(j)}\ .$$

Gauging condition

$$\boxed{\dot{\mathbf{b}}_\ell^{(\alpha)} \perp \mathbf{U}_\alpha, \text{i.e. } \dot{\mathbf{b}}_\ell^{(\alpha)} = P_\alpha^\perp \dot{\mathbf{b}}_\ell^{(\alpha)}}$$

$$P_\alpha : \mathbf{V}_\alpha \to \mathbf{U}_\alpha, \qquad P_\alpha = \sum_{\ell=1}^{r_\alpha} \left\langle \cdot, \mathbf{b}_\ell^{(\alpha)} \right\rangle \mathbf{b}_\ell^{(\alpha)} \quad P_\alpha^\perp := I - P_\alpha.$$

Local Parametrization. recursive describtion

Transport the parametrization of the tangent space onto a local parametrization of HT tensors with given ranks r_α

Let

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

be fixed . We define recursively

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

and

$$\widetilde{\mathbf{v}} = \sum_{i=1}^{r_D} (c_i^{(D)} + c_i^{(D)}) \widetilde{\mathbf{b}_i^{(D)}} \in U_\delta(\mathbf{v})$$

where $\delta c_{ij}^{(\alpha,\ell)} \perp c_{ij}^{(\alpha,\ell')}$ for all $\ell, \ell' = 1 \ldots, r_\alpha$.

Projection onto the tangent space

Let $\mathbf{v} \in \mathbf{V}$ be an HT tensor, $\alpha \subset D$, we decompose

$$\mathbf{v} = \sum_{\ell=1}^{r_\alpha} \mathbf{b}_\ell^{(\alpha)} \otimes \mathbf{w}_\ell^{(\alpha^C)} ,$$

with $\mathbf{w}_\ell^{(\alpha^C)} \in \mathbf{V}_{\alpha^C}$, $\alpha^C = D \backslash \alpha$, $\ell = 1, \ldots, r_\alpha$.

cutting leaves algorithm

An element $\delta\mathbf{v} \in \mathcal{T}_{\mathbf{v}}$ is of the form

$$\delta\mathbf{v} = \sum_{\ell=1}^{r_\alpha} (\delta\mathbf{b}_\ell^{(\alpha)} \otimes \mathbf{w}_\ell^{(\alpha^C)} + \mathbf{b}_\ell^{(\alpha)} \otimes \delta\mathbf{w}_\ell^{(\alpha^C)}) ,$$

where $\delta\mathbf{b}_\ell^{(\alpha)} \perp \mathbf{U}_\alpha$ and $\mathbf{w}_\ell^{(\alpha^C)}, \delta\mathbf{w}_\ell^{(\alpha^C)} \in \mathbf{V}_{\alpha^C}$, $\ell = 1, \ldots, r_\alpha$.

Retractions, extensions and density matrices for TT

Let $x_i \mapsto \mathbf{W}_i(x_i) \in \mathbb{R}^{r_{i-1} \cdot n_i \cdot r_i}$ be of the size of a component tensor. The extension or dressing operator

$$\mathbf{P}_{i,1,U} := \mathbf{E}_i := \mathbf{E}_i(U) : X \to \mathbb{T}_{\mathbf{r}} \subset \mathcal{H} ,$$

extending W_i to a TT tensor in $\mathcal{H} = \bigotimes_{i=1}^{d} \mathbb{R}^{n_i}$, is defined by

$$\mathbf{W}_i(x_i) \mapsto \mathbf{E}_i \mathbf{W}_i(\mathbf{x}) := \mathbf{U}_1(x_1) \cdots \mathbf{W}_i(x_i) \cdots \mathbf{U}_d(x_d) .$$

The adjoint operator is $\mathbf{E}_i^T$. $\mathbf{P}_{i,2,U} := \mathbf{E}_{i,i+1}$ is defined analogously.

The left inverse $\mathbf{E}_i^\dagger$ applied to the tensor $U = \mathbf{U}_1 \cdots \mathbf{U}_i \cdots \mathbf{U}_d \in \mathbb{T}_{\mathbf{r}}$ is given by

$$\mathbf{U}_i = \mathbf{E}_i^\dagger U = (\mathbf{E}_i^T \mathbf{E}_i)^{-1} \mathbf{E}_i^T U .$$

E.g, if $\mathbf{U}_i$, $i = 1, \ldots, d-1$, are left orthogonal, the $i-$th density matrix will be defined by

$$\mathbf{I} \otimes \mathbf{D}_i := (\mathbf{E}_i^T \mathbf{E}_i)^{-1} .$$

Projection to the tangent space

Let $U = \mathbf{U}_1 \cdots \mathbf{U}_i \cdots \mathbf{U}_d \in \mathbb{T}^{\mathbf{r}}$ be fixed, and
$\mathbf{U}_i$, $i = 1, \ldots, d-1$, are left orthogonal.
For $B \in \mathcal{H}$, the projection onto the tangent space $\mathcal{T}_U$ at $U \in \mathbb{T}_{\mathbf{r}}$ is given by

$$P_{\mathcal{T}_U} B = \mathbf{E}_d \mathbf{E}_d^T B + \sum_{i=1}^{d-1} \mathbf{E}_i \big((\mathbf{I} - \mathbf{P}_i) \otimes \mathbf{D}_i{}^{-1} \big) \mathbf{E}_i^T B \, .$$

where the orthogonal projection $\mathbf{P}_i$, to satisfy the gauge condition, is defined by

$$\mathbf{P}_i \mathbf{W}(k_{i-1}, x_i, k_i) = \sum_{k'_{i_1}, x'_i, k'_i} \mathbf{U}_i(k'_{i-1}, x'_i, k'_i) \mathbf{W}(k'_{i-1}, x'_i, k_i) \mathbf{U}_i(k_{i-1}, x_i, k'_i)$$

Let

$$\rho := \min\{\rho_i := \sigma_{i,r_i} : i = 1, \ldots, d-1\} ,$$

$\sigma_{i,\mu}$ are the singular values from matricisation $\mathbf{A}_i = U_{x_1,\ldots,x_i}^{x_{i+1},\ldots,x_d}$.

Lemma

$$cond\, \mathbf{D}_j = \rho_j^{-2} = \sigma_{j,r_j}^{-2} .$$

For the generalized inverse of $\mathbf{E}_j$

$$\|\mathbf{E}_j^{\dagger} B\| \le c\rho_j^{-1} \|U\| \|B\| , \; B \in \mathcal{H} .$$

Theorem (in prep.)

For $U, V \in \mathbb{T}_{\mathbf{r}}$ *and* $\|U - V\| \le c\rho$, $B \in \mathcal{H}$, *there exists* C *depending only on* n, d, *such that there holds*

$$\begin{aligned} \|\big(P_{\mathcal{T}(U)} - P_{\mathcal{T}(V)}\big)B\| &\le C\rho^{-1}\|U - V\|\|B\| \\ \|\big(I - P_{\mathcal{T}(U)}\big)(U - V)\| &\le C\rho^{-1}\|U - V\|^2 . \end{aligned}$$

These are estimates for the curvature of $\mathbb{T}_{\mathbf{r}}$.

Thank you
for your attention.

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