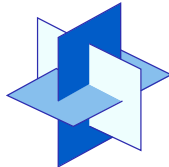
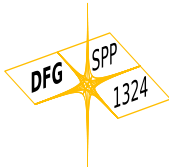


Manifolds and tangent spaces of TT and HT tensors

R. Schneider (TUB Matheon)

John von Neumann Lecture – TU Munich, 2012



Noteable special case of HT:

TT format (Oseledets & Tyrtysnikov, 2009)

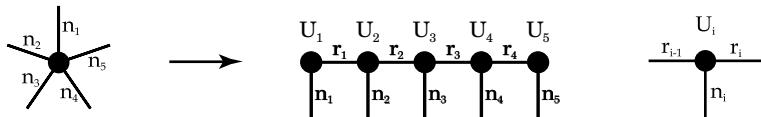
(matrix product states (MPS), Vidal 2003, Schöllwöck et al.)

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

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

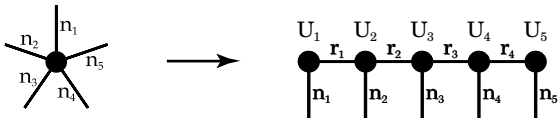
$$\mathbf{U} = (U_{k_1, \dots, k_d})_{k_i=0, 1 \leq i \leq d}^{n_i}$$

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

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

II.

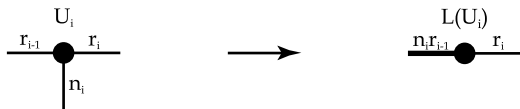
Existence and uniqueness results



Definitions: Left and right unfoldings

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

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



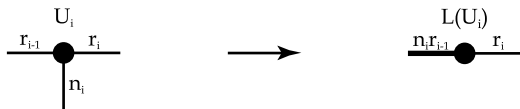
- ▶ **Left rank** of \mathbf{U}_i is $\text{rank } \mathbf{L}(\mathbf{U}_i(x_i))$,
- ▶ \mathbf{U}_i is **left orthogonal** if $\mathbf{L}(\mathbf{U}_i(x_i)) \in \mathcal{O}(\mathbb{R}^{(n_i r_{i-1}) \times r_i})$
- ▶ **Right** unfolding, right orthogonality, right rank: Via

$$\mathbf{R}(\mathbf{U}_i(x_i)) := U_{k_{i-1}}^{x_i, k_i}$$

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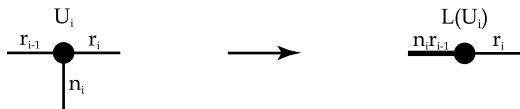
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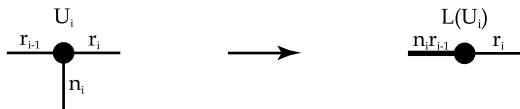
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Definitions: TT rank, separation rank

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

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

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

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

satisfy the full rank condition, the above decomposition is

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

i -th separation rank s_i of U :

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Existence and “uniqueness” of TT decompositions

Theorem (Holtz, R., Schneider, 2010)

- ▶ There is **exactly one rank vector** $\underline{r} = (r_1, \dots, r_{d-1})$ 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 $i = 1, \dots, d - 1$

- ▶ $r_i = s_j$ (separation ranks) for $i = 1, \dots, d - 1$

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

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

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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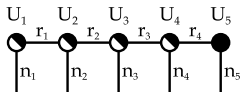
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III.

The manifold of tensors of fixed TT rank r

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



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

Theorem (Holtz, R. Schneider, 2010)

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

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

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

$$\delta U = \delta U_1 + \dots + \delta U_d$$

with

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

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

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

Sketch of proof

► Existence:

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

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

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

for $i = 1, \dots, d$, gauge condition (in other inner product) gives upper block- Δ -system with SPD matrices.

► $\mathbf{L}(\mathbf{W}_i)$, $i = d, d - 1, \dots, 1$ can uniquely be computed recursively.

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

- ▶ \mathcal{C}_i spaces of component functions \mathbf{U}_i , ($i = 1, \dots, d$)
- ▶ Left-orthonormal spaces of \mathbf{U}_i :

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

- ▶ Parameter space $X := U_1^\ell \times \dots \times U_{d-1}^\ell \times \mathcal{C}_d$.

Corollary (Holtz, R., Schneider, 2010)

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

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

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

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

Local parametrization for \mathbb{T}

Theorem (Holtz, R., Schneider, 2010)

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

$$\Psi(\mathbf{W}_1, \dots, \mathbf{W}_d) = (\mathbf{U}_1 + \mathbf{W}_1)(x_1) \cdots (\mathbf{U}_d + \mathbf{W}_d)(x_d).$$

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

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

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* $g = g_U : N_\delta \rightarrow \mathbb{R}^c$, $c = \sum_{i=1}^{d-1} r_i^2$, such that

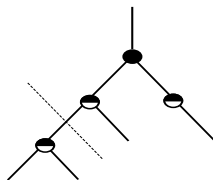
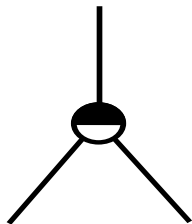
$$N_\delta \cap \mathbb{T} = \{U \in \mathbb{R}^{n^d} : g(U) = 0\} = \psi(N_\delta(0))$$

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

Hierarchical Tucker format: recursive description

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

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



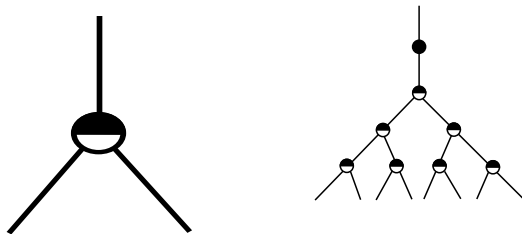
Coefficients $c_{ij}^{(\alpha, \ell)}$ form the matrices $C^{(\alpha, \ell)}$.

Final representation of \mathbf{v} is

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

Recursive description: 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 $\{C^{(\alpha, \ell)} : 1 \leq \ell \leq r_\alpha\}$ are orthonormal (w.r.t. the Frobenius scalar product).

Tangent tensors. recursive description

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

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

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

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

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

Gauging condition

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

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

Local Parametrization. recursive description

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

Let

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

be fixed . We define recursively

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

and

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

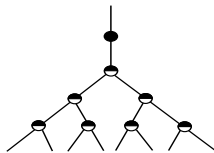
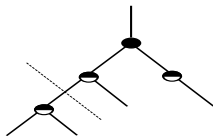
where $\delta c_{ij}^{(\alpha,\ell)} \perp c_{ij}^{(\alpha,\ell')}$ for all $\ell, \ell' = 1 \dots, r_\alpha$.

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 $\mathbf{w}_\ell^{(\alpha^C)} \in \mathbf{V}_{\alpha^C}$, $\alpha^C = D \setminus \alpha$, $\ell = 1, \dots, r_\alpha$.
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 $\mathbf{w}_\ell^{(\alpha^C)}, \delta \mathbf{w}_\ell^{(\alpha^C)} \in \mathbf{V}_{\alpha^C}$, $\ell = 1, \dots, r_\alpha$.

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**

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

extending \mathbf{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 $U = \mathbf{U}_1 \cdots \mathbf{U}_i \cdots \mathbf{U}_d \in \mathbb{T}_r$ 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 , $i = 1, \dots, d-1$, 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 $U = \mathbf{U}_1 \cdots \mathbf{U}_i \cdots \mathbf{U}_d \in \mathbb{T}^r$ be fixed, and

$\mathbf{U}_i, i = 1, \dots, d-1$, are left orthogonal.

For $B \in \mathcal{H}$, the projection onto the tangent space \mathcal{T}_U at $U \in \mathbb{T}^r$ is given by

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

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

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

Let

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

$\sigma_{i,\mu}$ are the singular values from matricisation $\mathbf{A}_i = U_{X_1, \dots, X_i}^{X_{i+1}, \dots, X_d}$.

Lemma

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

For the generalized inverse of \mathbf{E}_j

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

Theorem (in prep.)

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

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

These are estimates for the curvature of \mathbb{T}_r .

Thank you for your attention.

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