

Geometric structures and tensor based algorithms

Antonio Falcó



WORKSHOP NUMERICAL METHODS FOR HIGH-DIMENSIONAL
PROBLEMS

- 1 Algebraic and topological tensor spaces
- 2 Tensor based Banach manifolds
 - Algebraic and Topological Tree Based Tensors (TBT)
 - Main Results

- A. Falcó, W. Hackbusch and A. Nouy. Geometric Structures in Tensor Representations. Preprint 9/2013 at Max Planck Institute for Mathematics in the Sciences (2013).
- A. Falcó and W. Hackbusch. Minimal subspaces in tensor representations. Foundations of Computational Mathematics, Volume 12, Issue 6 (2012), pp 765-803 .

Algebraic tensor spaces

As a first example

$${}_a \bigotimes_{j=1}^d H^{N,p}(I_j) = \text{span} \underbrace{\{f_1(x_1) \cdots f_d(x_d) : f_i \in H^{N,p}(I_i)\}}_{\Sigma}$$

is a tensor space. In particular, we have

$${}_a \bigotimes_{j=1}^d L^p(I_j) = \text{span} \underbrace{\{f_1(x_1) \cdots f_d(x_d) : f_i \in L^p(I_i)\}}_{\Sigma}$$

for $1 \leq p < \infty$.

Topological tensor spaces

$$H^{N,p}(I_1 \times \cdots \times I_d) = \|\cdot\|_{N,p} \bigotimes_{j=1}^d H^{N,p}(I_j)$$

is a Banach tensor space $p \neq 2$ and a Hilbert tensor space for $p = 2$. In particular, we have

$$L^p(I_1 \times \cdots \times I_d) = \|\cdot\|_{0,p} \bigotimes_{j=1}^d L^p(I_j)$$

for $1 \leq p < \infty$. In general, for a norm $\|\cdot\|$ defined over an algebraic tensor space we will write:

$$\|\cdot\| \bigotimes_{j=1}^d V_j = \overline{\|\cdot\|} \bigotimes_{j=1}^d V_j, \quad V_j \text{ is a vector space !}$$

Definition

Take an algebraic tensor space $\mathbf{V}_D := {}_a \bigotimes_{j=1}^d V_j$ and fix some d -tuple $\mathbf{r} \in \mathbb{N}^d$. The set of tensors of bounded rank \mathbf{r} is defined by

$$\mathcal{T}_{\mathbf{r}}(\mathbf{V}_D) := \left\{ \mathbf{v} \in \mathbf{V}_D : \mathbf{v} \in {}_a \bigotimes_{j=1}^d U_j \quad \dim U_j \leq r_{\alpha} \text{ for all } j \right\}, \quad (1)$$

and the set of tensors of fixed rank \mathbf{r} is defined by

$$\mathcal{M}_{\mathbf{r}}(\mathbf{V}_D) := \{ \mathbf{v} \in \mathcal{T}_{\mathbf{r}}(\mathbf{V}_D) : \dim U_j = r_j \text{ for all } j \}. \quad (2)$$

The good, the bad and the ugly (Sergio Leone-1966)

Take $\mathbf{V}_{123} := V_1 \otimes_a V_2 \otimes_a V_3$ and a norm $\|\cdot\|_{23}$ defined over $\mathbf{V}_{23} := V_2 \otimes_a V_3$. Let $\|\cdot\|_{123}$ be a norm defined over $V_1 \otimes_a \overline{\mathbf{V}_{23}}^{\|\cdot\|_{23}}$. Then we have either

$$\mathcal{M}_r(\mathbf{V}_{123}) \subset \mathcal{T}_r(\mathbf{V}_{123}) \subset \mathbf{V}_{123} \subset \overline{V_1 \otimes_a \mathbf{V}_{23}}^{\|\cdot\|_{23}} \|\cdot\|_{123}$$

or

$$\mathcal{M}_r(\mathbf{V}_{123}) \subset \mathcal{T}_r(\mathbf{V}_{123}) \subset \mathbf{V}_{123} \subset \overline{V_1 \otimes_a \mathbf{V}_{23}}^{\|\cdot\|_{123}}$$

The best approximation and the geometric structure are norm dependent problems. The question is: Who is the good/bad/ugly?

The answer my friend is blowing in the wind (Bob Dylan)

- If V_i is a normed space with norm $\|\cdot\|_i$, then $\overline{V_i^{\|\cdot\|_i}}$ is always a Banach space, and then we have

$$\bigotimes_{j=1}^d V_j \subset \bigotimes_{j=1}^d \overline{V_i^{\|\cdot\|_i}} \quad \text{then} \quad \overline{\bigotimes_{j=1}^d V_j} \subset \overline{\bigotimes_{j=1}^d \overline{V_i^{\|\cdot\|_i}}}$$

- The equality (that always holds in finite dimension)

$$\overline{\bigotimes_{j=1}^d V_j} = \overline{\bigotimes_{j=1}^d \overline{V_i^{\|\cdot\|_i}}}$$

is true when the tensor product is continuous.

A desirable property

The equality is also true when $\|\cdot\| \gtrsim \|\cdot\|_{V(\bar{V}_1^{\|\cdot\|_1}, \dots, \bar{V}_d^{\|\cdot\|_d})}$. Clearly, the tensor product is continuous.

Definition (Injective norm)

Let V_i be a Banach spaces with norm $\|\cdot\|_i$ for $1 \leq i \leq d$. Then for $\mathbf{v} \in \mathbf{V} = {}_a \bigotimes_{j=1}^d V_j$ define $\|\cdot\|_{\mathbf{V}} = \|\cdot\|_{V(V_1, \dots, V_d)}$ by

$$\|\mathbf{v}\|_{\mathbf{V}} := \sup \left\{ \frac{|(\varphi_1 \otimes \varphi_2 \otimes \dots \otimes \varphi_d)(\mathbf{v})|}{\prod_{j=1}^d \|\varphi_j\|_j^*} : 0 \neq \varphi_j \in V_j^*, 1 \leq j \leq d \right\}.$$

Theorem (Best approximation)

Let V_i be a Banach spaces with norm $\|\cdot\|_i$, for $1 \leq i \leq d$. and let $\|\cdot\|$ be a norm on the algebraic tensor space $\mathbf{V}_D := {}_a \bigotimes_{j=1}^d V_j$. If

$\|\cdot\| \gtrsim \|\cdot\|_{V(V_1, \dots, V_d)}$ holds and $\overline{V}_D^{\|\cdot\|}$ is a reflexive Banach space. Then the set $\mathcal{T}_r(\mathbf{V}_D)$ is (weakly closed) proximal in $\overline{V}_D^{\|\cdot\|}$.

An optimization problem

Assume that there exists a manifold $\mathbb{M} = \mathcal{M}_r(\mathbf{V}_D) \subset \Sigma = \mathcal{T}_r(\mathbf{V}_D)$ such that

$$\min_{\mathbf{w} \in \Sigma} J(\mathbf{w}) = \min_{\mathbf{w} \in \mathbb{M}} J(\mathbf{w})$$

holds. Then $\mathbf{v} \in \arg \min_{\mathbf{w} \in \Sigma} J(\mathbf{w})$ satisfies the following first order condition (Euler-Lagrange Equation):

$$\langle J'(\mathbf{v}), \dot{\mathbf{w}} \rangle = 0 \text{ for all } \dot{\mathbf{w}} \in \mathbb{T}_{\mathbf{v}}\mathbb{M}.$$

Question

Is $\mathcal{M}_r(\mathbf{V}_D)$ a manifold? and a more important thing: Where is? (ambient space).

Tensor Based manifolds: Hartree Banach manifold

$$\mathbb{M}_{\text{Hartree}} = \{f_1(x_1) \cdots f_d(x_d) : f_i \in H^{N,p}(I_i) \setminus \{0\}\} \subset H^{N,p}(I_1 \times \cdots \times I_d)$$

The natural coordinates of $\mathbb{M}_{\text{Hartree}} = \mathcal{M}_{(1,\dots,1)}(a \otimes_{j=1}^d H^{1,p}(I_j))$

$$\mathbf{v} = \lambda f_1(x_1) \cdots f_d(x_d) = \lambda f_1 \otimes \cdots \otimes f_d,$$

are given as follows: Let $W_i(f_i) : H^{N,p}(I_i) = \text{span}\{f_i\} \oplus W_i(f_i)$ for $1 \leq i \leq d$. Then $\mathbf{v} + \delta\mathbf{v}$ is in a “natural neighborhood” of \mathbf{v} if and only if

$$\mathbf{v} + \delta\mathbf{v} = \eta (f_1 + \delta f_1)(x_1) \cdots (f_d + \delta f_d)(x_d) \quad \delta f_i \in W_i(f_i) \quad 1 \leq i \leq d.$$

So the “coordinates” of $\mathbf{v} + \delta\mathbf{v}$ are $(\eta, \delta f_1, \dots, \delta f_d)$ (for \mathbf{v} are $(\lambda, 0, \dots, 0)$).

Tangent space

Under this coordinates the “natural tangent space” at $\mathbf{v} = \lambda f_1 \otimes \cdots \otimes f_d$ is

$$\mathbb{T}_{\mathbf{v}}\mathbb{M}_{\text{Hartree}} = \mathbb{R} \times W_1(f_1) \times \cdots \times W_d(f_d),$$

that is, a velocity $\dot{\mathbf{v}}$ in $\mathbb{T}_{\mathbf{v}}\mathbb{M}_{\text{Hartree}}$ is given by

$$\dot{\mathbf{v}} \equiv (\eta, \delta f_1, \dots, \delta f_d).$$

Rank-one minimization

Since $\Sigma = \mathcal{T}_{(1, \dots, 1)}(a \otimes_{j=1}^d H^{1,p}(I_j)) = \overline{\mathbb{M}_{\text{Hartree}}}^{\|\cdot\|_{N,p}} \subset H^{N,p}(I_1 \times \dots \times I_d)$ is weakly closed, then the problem

$$\min_{\mathbf{w} \in \Sigma} J(\mathbf{w})$$

is well-posed. If $\mathbf{0} \neq \mathbf{v} \in \arg \min_{\mathbf{w} \in \Sigma} J(\mathbf{w})$, then

$$\min_{\mathbf{w} \in \Sigma} J(\mathbf{w}) = \min_{\mathbf{w} \in \mathbb{M}_{\text{Hartree}}} J(\mathbf{w}).$$

Find $\lambda f_1(x_1) \cdots f_d(x_d) \in \mathbb{M}_{\text{Hartree}}$:

$$\langle J'(\lambda f_1(x_1) \cdots f_d(x_d)), \dot{\mathbf{v}} \rangle = 0 \quad \dot{\mathbf{v}} \in \mathbb{R} \times W_1(f_1) \times \cdots \times W_d(f_d).$$

We need “to embed” $\dot{\mathbf{v}} \in \mathbb{R} \times W_1(f_1) \times \cdots \times W_d(f_d)$ into $H^{N,p}(I_1 \times \cdots \times I_d)$.

Embedding manifold

Let us consider the standard inclusion map (the identity)

$$i : \mathbb{M}_{\text{Hartree}} \rightarrow H^{N,p}(I_1 \times \cdots \times I_d), \quad \lambda f_1 \cdots f_d \mapsto \lambda \bigotimes_{i=1}^d f_i.$$

In local coordinates is a map $(i \circ \varphi_{\mathbf{v}}^{-1}) :$

$(\mathbb{R} \setminus \{0\}) \times W_1(f_1) \times \cdots \times W_d(f_d) \rightarrow H^{N,p}(I_1 \times \cdots \times I_d)$ given by

$$(\eta, \delta f_1, \dots, \delta f_d) \mapsto \eta (f_1 + \delta f_1) \cdots (f_d + \delta f_d).$$

Its derivative $T_{\mathbf{v}}i := (i \circ \varphi_{\mathbf{v}}^{-1})'(\lambda, 0, \dots, 0)$ is a linear map given by

$$T_{\mathbf{v}}i(\gamma, \delta f_1, \dots, \delta f_d) = \gamma \bigotimes_{i=1}^d f_j + \sum_{j=1}^d \lambda \delta f_j \otimes \bigotimes_{k \neq j} f_k.$$

Is an embedding manifold ?

- Is $T_{\mathbf{v}}i : \mathbb{R} \times W_1(f_1) \times \cdots \times W_d(f_d) \rightarrow H^{N,p}(I_1 \times \cdots \times I_d)$ injective ?
- Is the linear subspace $T_{\mathbf{v}}i(\mathbb{R} \times W_1(f_1) \times \cdots \times W_d(f_d)) = \mathbf{Z}(\mathbf{v})$ where

$$\mathbf{Z}(\mathbf{v}) := \left\{ \gamma \bigotimes_{i=1}^d f_j + \sum_{j=1}^d \lambda \delta f_j \otimes \bigotimes_{k \neq j} f_k : \begin{array}{l} (\gamma, \delta f_1, \dots, \delta f_d) \\ \in T_{\mathbf{v}}\mathbb{M}_{\text{Hartree}} \end{array} \right\}$$

closed and complemented in $H^{N,p}(I_1 \times \cdots \times I_d)$?

- Observe that the subspace

$$\mathbf{Z}(\mathbf{v}) = \bigotimes_{i=1}^d \text{span}\{f_i\} \oplus \left(\bigoplus_{j=1}^d W_j(f_j) \otimes_a \text{span}\{\lambda \bigotimes_{k \neq j} f_k\} \right).$$

The answer my friend is blowing in the wind (Bob Dylan)

- If the tensor product \otimes is continuous then $T_{\mathbf{v}}j$ is well defined and it is also injective.

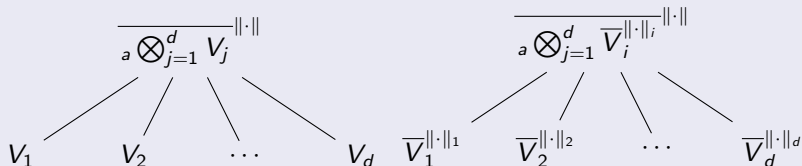
Theorem

Let V_i be a Banach spaces with norm $\|\cdot\|_i$ for $1 \leq i \leq d$. and let $\|\cdot\|$ be a norm on the algebraic tensor space $\mathbf{V}_D := {}_a \otimes_{j=1}^d V_j$. If $\|\cdot\| \gtrsim \|\cdot\|_{V(V_1, \dots, V_d)}$ holds then for each $\mathbf{v} \in \mathcal{M}_r(\mathbf{V}_D)$ the linear subspace $\mathbf{Z}(\mathbf{v})$ is closed and complemented in $\overline{\mathbf{V}_D}^{\|\cdot\|}$, and hence $\mathcal{M}_r(\mathbf{V}_D)$ is a submanifold of $\overline{\mathbf{V}_D}^{\|\cdot\|}$.

Comments

- The manifold of tensors of fixed rank is an analytical Banach manifold even if the tensor product map is not continuous.
- If the tensor product map is continuous then (i) we can compute T_i in order to transport velocities and (ii) the tangent space can be identify with a linear space $\mathbf{Z}(\mathbf{v})$ inside the tensor Banach space.
- If $\|\cdot\| \gtrsim \|\cdot\|_{\mathbf{V}(v_1, \dots, v_d)}$ holds then the manifold of tensor of fixed rank is a submanifold inside the tensor Banach space.

The moral of the tale



both tensor representations are the same when $\|\cdot\| \gtrsim \|\cdot\|_V$ and the existence of a best approximation holds. We assume a tensor representation like

$$\mathbf{v} = \sum_{i_1=1}^{r_1} \cdots \sum_{i_d=1}^{r_d} C_{i_1 \dots i_d} \mathbf{u}_{i_1} \otimes \cdots \otimes \mathbf{u}_{i_d}$$

where $C_{i_1 \dots i_d} \in \mathbb{R}^{r_1 \times \dots \times r_d}$ and $\{\mathbf{u}_{i_k}\}_{i_k=1}^{i_k=r_k}$ is a basis of a subspace U_k in V_k for $1 \leq k \leq d$. So $\mathbf{v} \in a \otimes_{k=1}^d U_k$ and $\text{rank } \mathbf{v} = (r_1, \dots, r_d)$.

Algebraic Tree Based Tensors

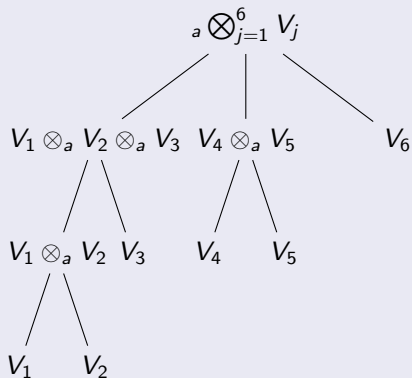
Take $D = \{1, 2, \dots, d\}$ be the root then a tree T_D is defined by

$$\mathbf{V}_D := {}_a \bigotimes_{\alpha \in S(D)} \mathbf{V}_\alpha = {}_a \bigotimes_{\alpha \in S(D)} \left({}_a \bigotimes_{\beta \in S(\alpha)} \mathbf{V}_\beta \right) = \dots = {}_a \bigotimes_{j \in D} V_j$$

where for $\delta \in 2^D \setminus \{\emptyset\}$ we put

$$\mathbf{V}_\delta := {}_a \bigotimes_{j \in \delta} V_j$$

Algebraic Tree Based Representation



Tensor representation

$$\mathbf{v} = \sum_{i_{123}=1}^{r_{123}} \sum_{i_{45}=1}^{r_{45}} \sum_{i_6=1}^{r_6} C_{i_{123}i_{45}i_6} \mathbf{u}_{i_{123}} \otimes \mathbf{u}_{i_{45}} \otimes u_{i_6}$$

where

$$\mathbf{u}_{i_{123}} = \sum_{i_{12}=1}^{r_{12}} \sum_{i_3=1}^{r_3} C_{i_{123};i_{12}i_3} \mathbf{u}_{i_{12}} \otimes u_{i_3},$$

$$\mathbf{u}_{i_{12}} = \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} C_{i_{12};i_1i_2} u_{i_1} \otimes u_{i_2},$$

and

$$\mathbf{u}_{i_{45}} = \sum_{i_4=1}^{r_4} \sum_{i_5=1}^{r_5} C_{i_{45};i_4i_5} u_{i_4} \otimes u_{i_5}.$$

Now the rank $\mathbf{v} = (r_{123}, r_{45}, r_6, r_{12}, r_3, r_4, r_5, r_1, r_2)$

Definition

Let T_D be a given dimension partition tree and fix some tuple $\tau \in \mathbb{N}^{T_D}$ for T_D . The set of TBF tensors of bounded TB rank τ is defined by

$$\mathcal{BT}_\tau(\mathbf{V}_D) := \{ \mathbf{v} \in \mathbf{V}_D : \dim U_\alpha^{\min}(\mathbf{v}) \leq r_\alpha \text{ for all } \alpha \in T_D \}, \quad (3)$$

and the set of TBF tensors of fixed TB rank τ is defined by

$$\mathcal{FT}_\tau(\mathbf{V}_D) := \{ \mathbf{v} \in \mathcal{BT}_\tau(\mathbf{V}_D) : \dim U_\alpha^{\min}(\mathbf{v}) = r_\alpha \text{ for all } \alpha \in T_D \}. \quad (4)$$

Remark

$$\mathcal{BT}_\tau(\mathbf{V}_D) = \bigcup_{\mathfrak{s} \leq \tau} \mathcal{FT}_\mathfrak{s}(\mathbf{V}_D)$$

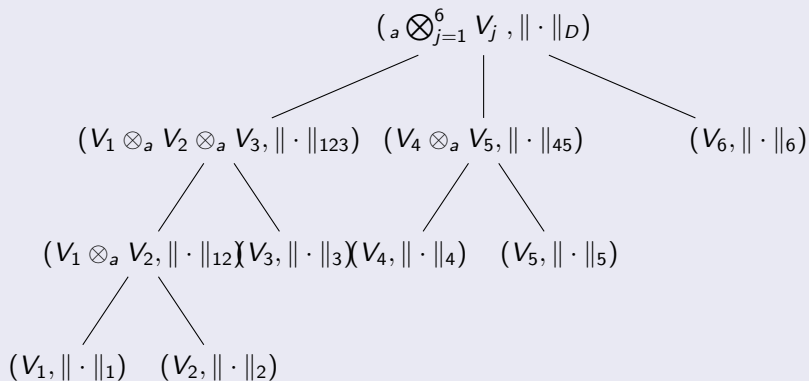
Property

Assume that $\mathbf{v} \in \mathcal{FT}_r(\mathbf{V}_D)$ then for each $\alpha \in T_D \setminus \{\{1\}, \dots, \{d\}\}$ it can be show that

$$C_{i_\alpha; (i_\beta)_{\beta \in S(\alpha)}} \in \mathbb{R}_*^{r_\alpha \times (\prod_{\beta \in S(\alpha)} r_\beta)},$$

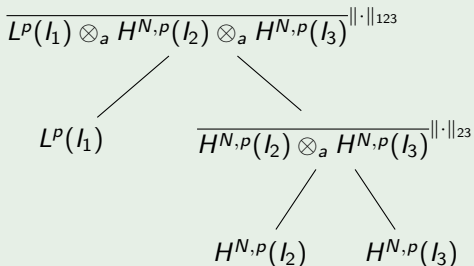
that is, $\text{rank } \mathcal{M}_\alpha(C_{i_\alpha; (i_\beta)_{\beta \in S(\alpha)}}) = r_\alpha$ and $\text{rank } \mathcal{M}_\beta(C_{i_\alpha; (i_\beta)_{\beta \in S(\alpha)}}) = r_\beta$ for all $\beta \in S(\alpha)$. Here rank means matrix rank and \mathcal{M}_β is the matricization of the tensor with respect the index β .

Topological Tree Based representation



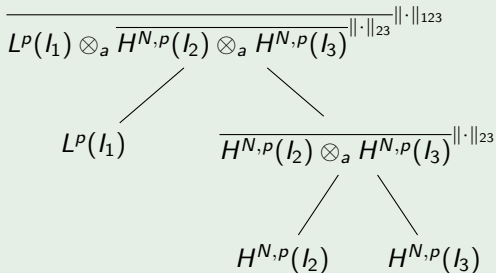
Example

Representation on topological tree based format



Example

No representation on topological tree based format



However, if $\|\cdot\|_{123} \gtrsim \|\cdot\|_{\vee(L^p(I_1), \overline{H^{N,p}(I_2) \otimes_a H^{N,p}(I_3)})^{\|\cdot\|_{23}}}$ holds both trees give the same representation.

Banach-Grassmann Manifold (A. Douady-1961)

For each $\alpha \in T_D \setminus \{D\}$, there exists $W_\alpha^{\min}(\mathbf{v})$ such that

$$\mathbf{V}_{\alpha_{\|\cdot\|_\alpha}} = U_\alpha^{\min}(\mathbf{v}) \oplus W_\alpha^{\min}(\mathbf{v})$$

Every U such that

$$\mathbf{V}_{\alpha_{\|\cdot\|_\alpha}} = U \oplus W_\alpha^{\min}(\mathbf{v})$$

is characterized by the existence of a unique $L_\alpha \in \mathcal{L}(U_\alpha^{\min}(\mathbf{v}), W_\alpha^{\min}(\mathbf{v}))$ such that

$$U = \text{span} \{ \mathbf{u}_{i_\alpha} + L_\alpha(\mathbf{u}_{i_\alpha}) : 1 \leq i_\alpha \leq r_\alpha \},$$

where

$$U_\alpha^{\min}(\mathbf{v}) = \text{span} \{ \mathbf{u}_{i_\alpha} : 1 \leq i_\alpha \leq r_\alpha \}.$$

Theorem

The set $\mathcal{FT}_\tau(\mathbf{V}_D)$ of TBF tensors with fixed TB rank is an analytical Banach manifold. **This geometric structure is independent of the choice of the norm $\|\cdot\|_D$.**

Example

Let $V_{1\|\cdot\|_1} := H^{1,p}(I_1)$ and $V_{2\|\cdot\|_2} = H^{1,p}(I_2)$. Take $\mathbf{V}_D := H^{1,p}(I_1) \otimes_a H^{1,p}(I_2)$, from Theorem 8 we obtain that $\mathcal{FT}_\tau(\mathbf{V}_D)$ is a Banach manifold. However, we can consider as ambient manifold either $\overline{\mathbf{V}}_D^{\|\cdot\|_{D,1}} := H^{1,p}(I_1 \times I_2)$ or $\overline{\mathbf{V}}_D^{\|\cdot\|_{D,2}} = H^{1,p}(I_1) \otimes_{\|\cdot\|_{(0,1),p}} H^{1,p}(I_2)$, where $\|\cdot\|_{(0,1),p}$ is the norm given by

$$\|f\|_{(0,1),p} := \left(\|f\|_p^p + \left\| \frac{\partial f}{\partial x_1} \right\|_p^p \right)^{1/p}$$

for $1 \leq p < \infty$.

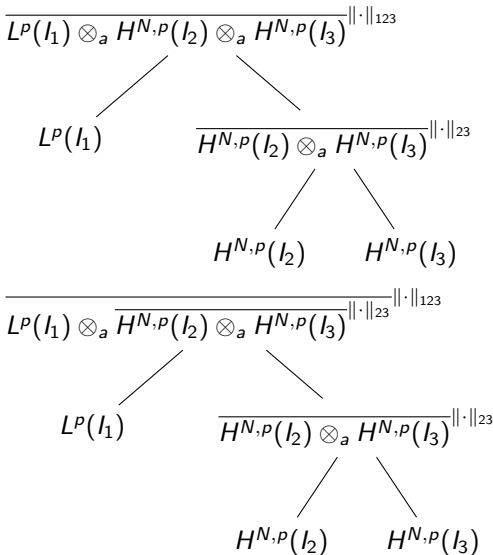
Assumption

$$\|\cdot\|_\alpha \gtrsim \|\cdot\|_{V(S(\alpha))} \text{ for each } \alpha \in \mathcal{T}_D \setminus \mathcal{L}(\mathcal{T}_D), \quad (5)$$

Theorem

Let $\{\mathbf{V}_{\alpha_{\|\cdot\|_\alpha}}\}_{\alpha \in \mathcal{T}_D \setminus \{D\}}$ be a representation of a tensor Banach space $\mathbf{V}_{D_{\|\cdot\|_D}} = \|\cdot\|_D \otimes_{j \in D} V_j$, in topological tree based format and assume that (5) holds. Then $\mathcal{FT}_\tau(\mathbf{V}_D)$ is an embedded submanifold of $\mathbf{V}_{D_{\|\cdot\|_D}}$. Moreover, we can construct a complemented subspace $\mathbf{Z}^{(D)}(\mathbf{v})$ such that $\mathbf{Z}^{(D)}(\mathbf{v}) = \mathbb{T}_{\mathbf{v}}i(\mathbb{T}_{\mathbf{v}}(\mathcal{FT}_\tau(\mathbf{V}_D)))$ holds for $\mathbf{v} \in \mathcal{FT}_\tau(\mathbf{V}_D)$.

If (5) holds then both trees are the same



Theorem

Let $\{\mathbf{V}_{\alpha\|\cdot\|\alpha}\}_{\alpha \in T_D \setminus \{D\}}$ be a representation of a reflexive Banach tensor space $\mathbf{V}_{D\|\cdot\|_D} = \|\cdot\|_D \otimes_{j \in D} V_j$, in topological tree based format and assume that (5) holds. Then for each $\mathbf{v} \in \mathbf{V}_{D\|\cdot\|_D}$ there exists $\mathbf{u}_{best} \in \mathcal{BT}_\tau(\mathbf{V}_D)$ such that

$$\|\mathbf{v} - \mathbf{u}_{best}\|_D = \min_{\mathbf{u} \in \mathcal{BT}_\tau(\mathbf{V}_D)} \|\mathbf{v} - \mathbf{u}\|_D,$$

here $\mathbf{V}_D = {}_a \otimes_{j \in D} V_j$.

Thank you for your attention !