Manifolds and tangent spaces of TT and HT tensors

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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

$$U(x) = U_1(x_1) \cdots U_i(x_i) \cdots U_d(x_d)$$

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

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

Redundancy: $U(x) = U_1(x_1)GG^{-1}U_2(x_2) \cdots U_i(x_i) \cdots U_d(x_d)$. 
Setting - Tensors

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

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

The function \( U \in \mathcal{H} \) will be called an \textit{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 \textit{variables or indices}.

\[ k \mapsto U(k_1, \ldots, k_d) = (U_{k_1, \ldots, k_d}) , \quad k_i = 1, \ldots, n_i . \]

Or in index (vectorial) notation

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

\[ \dim \mathcal{H} = n^d \text{ \textit{curse of dimensions!!}} \]

E.g. wave function \( \psi(r_1, s_1, \ldots, r_N, s_N) \)
II. Existence and uniqueness results
Definitions: Left and right unfoldings

- **Left unfolding** of comp. functions \( U_i : x_i \to U_i(x_i) \in \mathbb{R}^{r_{i-1} \times r_i} : \\
Matrix \]

\[
L(U_i(x_i)) := U_{x_i,k_{i-1}}^{k_i} \in \mathbb{R}^{(r_{i-1}n_i) \times r_i}
\]

- **Left rank** of \( U_i \) is rank \( L(U_i(x_i)) \),

- \( U_i \) is **left orthogonal** if \( L(U_i(x_i)) \in O(\mathbb{R}^{(n_ir_{i-1}) \times r_i}) \),

- **Right unfolding**, **right orthogonality**, **right rank**: Via

\[
R(U(x_i)) := U_{k_i-1}^{x_i,k_i}
\]
Definitions: Left and right unfoldings

- **Left unfolding** of comp. functions \( U_i : x_i \rightarrow U_i(x_i) \in \mathbb{R}^{r_i-1 \times r_i} : \

  \text{Matrix} \quad \mathbf{L}(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 \( U_i \) is \( \text{rank} \mathbf{L}(U_i(x_i)) \).

- **\( U_i \) is left orthogonal** if \( \mathbf{L}(U_i(x_i)) \in O(\mathbb{R}^{(n_i,r_i-1) \times r_i}) \).

- **Right unfolding**, **right orthogonality**, **right rank**: Via

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- **Left rank** of $U_i$ is rank $L(U_i(x_i))$,

- $U_i$ is **left orthogonal** if $L(U_i(x_i)) \in \mathcal{O}(\mathbb{R}^{(n_i r_{i-1}) \times r_i})$

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  $$R(U(x_i)) := U_{k_i-1}^{x_i,k_i}.$$
Definitions: TT rank, separation rank

\( U_i(x_i) : \{1, \ldots, n_i\} \rightarrow \mathbb{R}^{r_{i-1} \times r_i} \) satisfies full rank condition iff

\[
\text{rank } L(U_i(x_i)) = r_i = \text{rank } R(U_{i+1}(x_{i+1})).
\]

If all component functions \( U_i(x_i) \) of a TT decomposition

\[
U(x) = U_1(x_1)U_2(x_2) \ldots \ldots U_{d-1}(x_{d-1})U_d(x_d)
\]

satisfy the full rank condition, the above decomposition is a decomposition of TT rank \( r = (r_1, \ldots, r_{d-1}) \).

\( i \)-th seperation rank \( s_i \) of \( U \):

\[
\text{Rank of } A_i = U_{x_1,\ldots,x_i}^{x_{i+1},\ldots,d}.
\]
Definitions: TT rank, separation rank

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\[ i\text{-th separation rank } s_i \text{ of } U: \]

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\text{Rank of } A_i = U_{x_1, \ldots, x_i}^{x_{i+1}, \ldots, d}.
\]
Existence and “uniqueness” of TT decompositions

Theorem (Holtz, R., Schneider, 2010)

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

  For other TT decompositions, \( r'_i \geq r_i \) for all \( i = 1, \ldots, d - 1 \)

- \( r_i = s_i \) (separation ranks) for \( i = 1, \ldots, d - 1 \)

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

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

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

\[
\mathbf{U}_1(x_1)\mathbf{Q}_1 = \mathbf{V}_1(x_1), \quad \mathbf{Q}^T_{d-1}\mathbf{U}_d(x_d) = \mathbf{V}_d(x_d),
\]

\[
\mathbf{Q}^T_{i-1}\mathbf{U}_i(x_i)\mathbf{Q}_i = \mathbf{V}_i(x_i).
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U_1(x_1) \cdots U_i(x_i) \cdots U_d(x_d) = V_1(x_1) \cdots V_i(x_i) \cdots V_d(x_d)
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iff for some \( Q_i \in \mathcal{O}(\mathbb{R}^{r_i \times r_i}) \),

\[
U_1(x_1)Q_1 = V_1(x_1), \quad Q_{d-1}^T U_d(x_d) = V_d(x_d),
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\[
Q_{i-1}^T U_i(x_i)Q_i = V_i(x_i).
\]
Existence and “uniqueness” of TT decompositions

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

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

  $$U_1(x_1) \cdots U_i(x_i) \cdots U_d(x_d) = V_1(x_1) \cdots V_i(x_i) \cdots V_d(x_d)$$

  iff for some $Q_i \in O(\mathbb{R}^{r_i \times r_i})$,

  $$U_1(x_1)Q_1 = V_1(x_1), \quad Q_{d-1}^T U_d(x_d) = V_d(x_d),$$

  $$Q_{i-1}^T U_i(x_i)Q_i = V_i(x_i).$$
Principle bundle

Consider the (linear) parameter space

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

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

\[ G_i U_i := G_{i-1}^{-1} U_i(x_i) G_i , \quad i = 1, \ldots, d - 1, \quad U_i \in X_i . \]

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

And define the Lie group

\[ G \in G_r := \times_{i=1}^{d-1} GL(R^{r_i}) , \quad G_r U := (G_i U_i)_{i=1}^{d} \]

this but induces an equivalence relation

\[ U \sim V \iff U = GV , \quad G \in G_r \]

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

\[ \mathcal{M}_r \simeq ( \times_{i=1}^{d} X_i ) / G_r \]
III.

The manifold of tensors of fixed TT rank $r$

\[ \mathbb{T} := \mathbb{T}_r := \{ U \in \mathbb{R}^{n_1 \times \ldots \times n_d} \text{ tensor of TT rank } r \} .\]
Unique representation of the tangent space of $\mathbb{T}$

Theorem (Holtz, R. Schneider, 2010)

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

$$
\delta U \in T_{\mathcal{U}} \mathbb{T} \simeq \left\{ \gamma'(t)|_{t=0} \mid \gamma \in C^1([\delta, \delta], \mathbb{R}), \right. \\
\gamma(t) = U_1(x_1, t) \cdots U_d(x_d, t), \quad \gamma(0) = U(x) \left\}
$$

there is a unique vector $(W_1, \ldots, W_d)$ of component functions $W_i(\cdot) : I_i \rightarrow \mathbb{R}^{r_{i-1} \times r_i}$, such that

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

with

$$
\delta U_i := U_1(x_1) \cdots U_{i-1}(x_{i-1}) W_i(x_i) U_{i+1}(x_{i+1}) \cdots U_d(x_d),
$$

and s.t. $W_i(\cdot)$ fulfil the (left-orthogonality) gauge conditions

$$
L(U_i)^T L(W_i) = 0 \in \mathbb{R}^{r_i \times r_i} \text{ for } i = 1, \ldots, d - 1.
$$
Sketch of proof

- **Existence:**
  \[
  \delta U \simeq U'_1(x_1, 0)U_2(x_2)\cdots U_d(x_d) + U_1(x_1)U'_2(x_2, 0)\cdots U_d(x_d) + \cdots + U_1(x_1)\cdots U_{d-1}(x_{d-1})U'_d(x_d, 0).
  \]
  Left orthogonal decomposition: there exists unique \( \Lambda_1 \) s.t.
  \[
  U'(x_1, 0) = U_1(x_1)\Lambda_1 + W_1(x_1),
  \]
  iterate.

- **Uniqueness:** (Idea from Lubich et al., Tucker format)
  - Testing \( \delta U \) with
    \[
    V_i(x) := U_1(x_1)\cdots U_{i-1}(x_{i-1})V_i(x_i)U_{i+1}(x_{i+1})\cdots U_d(x_d),
    \]
    for \( i = 1, \ldots, d \), gauge condition (in other inner product) gives upper block-\( \Delta \)-system with SPD matrices.
  - \( L(W_i), i = d, d-1, \ldots, 1 \) can uniquely be computed recursively.
Parametrization of $\mathcal{T}_U \mathbb{T}$

- $C_i$ spaces of component functions $U_i$, $(i = 1, \ldots, d)$
- Left-orthonormal spaces of $U_i$:
  \[ U_i^\ell := \{ W_i(x_i) \in C_i, \quad L(U_i)^T L(W_i) = 0 \}. \]
- Parameter space $X := U_1^\ell \times \ldots \times U_{d-1}^\ell \times C_d$.

**Corollary (Holtz, R., Schneider, 2010)**

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

\[ \tau(W_1, \ldots, W_d) = \sum_{i=1}^{d} U_1 \cdots U_{i-1} W_i U_{i+1} \cdots U_d \]

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

$$
\Psi(W_1, \ldots, W_d) = (U_1 + W_1)(x_1) \cdot \ldots \cdot (U_d + W_d)(x_d).
$$

- There exists open $N_\delta(0) \subseteq \mathbb{R}^{\dim X}$ such that
  
  $\Psi|_{N_\delta} : N_\delta(0) \mapsto \Psi(N_\delta(0))$ 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

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

**Proof:** Inv. mapping theorem for manifolds, tang. space par. $\tau$
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

\[ \{ b_i^{(\alpha)} : 1 \leq i \leq r_\alpha \} \text{ orthonormal basis for } \alpha \in T_D. \]

This is equivalent to

1) At the leaves (\( \alpha = \{ j \}, j \in D \)): \( \{ b_i^{(j)} : 1 \leq i \leq r_j \} \) is chosen orthonormal.
2) The matrices \( \{ C^{(\alpha, \ell)} : 1 \leq \ell \leq r_\alpha \} \) are orthonormal (w.r.t. the Frobenius scalar product).
Let \( v(t) \) be a differentiable function. We characterise \( \dot{v}(t) \) at \( t = 0 \) and abbreviate \( \dot{v} := \dot{v}(0) \), \( (r_D = 1) \),

\[
\dot{v} = \dot{c}_1^{(D)} b_1^{(D)} + c_1^{(D)} \dot{b}_1^{(D)}.
\]

\[
\dot{b}_{\ell}^{(x)} = \sum_{i=1}^{r_{\alpha_1}} \sum_{j=1}^{r_{\alpha_2}} \dot{c}_{ij}^{(x,\ell)} b_i^{(\alpha_1)} \otimes b_j^{(\alpha_2)} + \sum_{i=1}^{r_{\alpha_1}} \sum_{j=1}^{r_{\alpha_2}} c_{ij}^{(x,\ell)} b_i^{(\alpha_1)} \otimes \dot{b}_j^{(\alpha_2)} + \sum_{i=1}^{r_{\alpha_1}} \sum_{j=1}^{r_{\alpha_2}} c_{ij}^{(x,\ell)} \dot{b}_i^{(\alpha_1)} \otimes b_j^{(\alpha_2)}
\]

\( \dot{v} \) is recursively determined by

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

**Gauging condition**

\[
\dot{b}_{\ell}^{(x)} \perp U_\alpha, \text{ i.e. } \dot{b}_{\ell}^{(x)} = P_\alpha \perp \dot{b}_{\ell}^{(x)}
\]

\[
P_\alpha : V_\alpha \rightarrow U_\alpha, \quad P_\alpha = \sum_{\ell=1}^{r_\alpha} \left\langle \cdot, b_{\ell}^{(x)} \right\rangle b_{\ell}^{(x)} \quad P_\alpha^\perp := I - P_\alpha.
\]
Local Parametrization. recursive description

Transport the parametrization of the tangent space onto a local parametrization of HT tensors with given ranks $r_\alpha$.

Let

$$U_\alpha = \text{span}\{b_i^{(\alpha)} : 1 \leq i \leq r_\alpha\}$$

be fixed. We define recursively

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

and

$$\tilde{v} = \sum_{i=1}^{r_D} (c_i^{(D)} + c_i^{(D)}) b_i^{(D)} \in U_\delta(v)$$

where $\delta c_{ij}^{(\alpha,\ell)} \perp c_{ij}^{(\alpha,\ell')} \text{ for all } \ell, \ell' = 1 \ldots, r_\alpha.$
Projection onto the tangent space

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

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

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

cutting leaves algorithm

An element $\delta v \in T_v$ is of the form

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

where $\delta b^{(\alpha)}_\ell \perp U_\alpha$ and $w^{(\alpha^C)}_\ell, \delta w^{(\alpha^C)}_\ell \in V_{\alpha^C}$, $\ell = 1, \ldots, r_\alpha$. 
Retractions, extensions and density matrices for TT

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

\[
P_{i,1,U} := E_i := E_i(U) : X \rightarrow \mathbb{T}_r \subset \mathcal{H},
\]

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

\[
W_i(x_i) \mapsto E_i W_i(x) := U_1(x_1) \cdots W_i(x_i) \cdots U_d(x_d).
\]

The adjoint operator is \( E_i^T \). \( P_{i,2,U} := E_{i,i+1} \) is defined analogously.

The left inverse \( E_i^\dagger \) applied to the tensor

\( U = U_1 \cdots U_i \cdots U_d \in \mathbb{T}_r \) is given by

\[
U_i = E_i^\dagger U = (E_i^T E_i)^{-1} E_i^T U.
\]

E.g., if \( U_i, i = 1, \ldots, d - 1, \) are left orthogonal, the \( i \)-th density matrix will be defined by

\[
I \otimes D_i := (E_i^T E_i)^{-1}.
\]
Projection to the tangent space

Let $U = U_1 \cdots U_i \cdots U_d \in T^r$ be fixed, and $U_i, i = 1, \ldots, d - 1$, are left orthogonal.

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

$$P_{T_U} B = E_d E_d^T B + \sum_{i=1}^{d-1} E_i ((I - P_i) \otimes D_i^{-1}) E_i^T B,$$

where the orthogonal projection $P_i$, to satisfy the gauge condition, is defined by

$$P_i W(k_{i-1}, x_i, k_i) = \sum_{k_i', x_i', k_i'} U_i(k_{i-1}', x_i', k_i') W(k_{i-1}', x_i', k_i) U_i(k_{i-1}, x_i, k_i')$$
Let
\[ \rho := \min \{ \rho_i := \sigma_{i,r_i} : i = 1, \ldots, d - 1 \} , \]
\( \sigma_{i,\mu} \) are the singular values from matricisation \( A_i = U_{x_1, \ldots, x_i}^{x_i+1, \ldots, x_d} \).

**Lemma**

\[ \text{cond } D_j = \rho_j^{-2} = \sigma_{j,r_j}^{-2} . \]

For the generalized inverse of \( E_j \)
\[ \| E_j^\dagger B \| \leq c \rho_j^{-1} \| U \| \| B \| , \quad B \in \mathcal{H} . \]

**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
\[ \| (P_{\mathbb{T}(U)} - P_{\mathbb{T}(V)}) B \| \leq C \rho^{-1} \| U - V \| \| B \| \]
\[ \| (I - P_{\mathbb{T}(U)})(U - V) \| \leq C \rho^{-1} \| U - V \|^2 . \]

These are estimates for the curvature of \( \mathbb{T}_r \).
Thank you for your attention.

References:

UNDER CONSTRUCTION,


I do not have suff. complete knowledge about physics literatur