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„Extraktion quantifizierbarer Information aus komplexen Systemen"

# On Manifolds of Tensors of Fixed TT-Rank 

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# ON MANIFOLDS OF TENSORS OF FIXED TT-RANK 

SEBASTIAN HOLTZ, THORSTEN ROHWEDDER, AND REINHOLD SCHNEIDER


#### Abstract

Recently, the format of TT tensors [19, 38, 34, 39] has turned out to be a promising new format for the approximation of solutions of high dimensional problems. In this paper, we prove some new results for the TT representation of a tensor $U \in$ $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ and for the manifold of tensors of TT-rank $\underline{r}$. As a first result, we prove that the TT (or compression) ranks $r_{i}$ of a tensor $U$ are unique and equal to the respective seperation ranks of $U$ if the components of the TT decomposition are required to fulfil a certain maximal rank condition. We then show that the set $\mathbb{T}$ of TT tensors of fixed rank $\underline{r}$ forms an embedded manifold in $\mathbb{R}^{n^{d}}$, therefore preserving the essential theoretical properties of the Tucker format, but often showing an improved scaling behaviour. Extending a similar approach for matrices [7], we introduce certain gauge conditions to obtain a unique representation of the tangent space $\mathcal{T}_{U} \mathbb{T}$ of $\mathbb{T}$ and deduce a local parametrization of the TT manifold. The parametrisation of $\mathcal{T}_{U} \mathbb{T}$ is often crucial for an algorithmic treatment of high-dimensional time-dependent PDEs and minimisation problems [33]. We conclude with remarks on those applications and present some numerical examples.


## 1. Introduction

The treatment of high-dimensional problems, typically of problems involving quantities from $\mathbb{R}^{d}$ for larger dimensions $d$, is still a challenging task for numerical approximation. This is owed to the principal problem that classical approaches for their treatment normally scale exponentially in the dimension $d$ in both needed storage and computational time and thus quickly become computationally infeasable for sensible discretizations of problems of interest. To circumvent this "curse of dimensionality" [5], alternative paradigms in their treatment are needed. Recent developments, motivated by problems in data compression and data analysis, indicate that concepts of tensor product approximation, i.e. the approximation of multivariate functions depending on $d$ variables $x_{1}, \ldots, x_{d}$ by sums and products of lower-dimensional quantities, often offer a flexible tool for the

[^0]data sparse approximation of quantities of interest.
In particular, this approach sheds new perspectives on the numerical treatment of PDEs in high dimensions, turning up in various applications from natural sciences as for example in the simulation of chemical reactions and in quantum dynamics, in the treatment of the Fokker-Planck equation or of boundary value problems with stochastic data. In particular, the treatment of the stationary electronic Schrödinger equation has recently received a lot of attention. In this case, the incorporation of antisymmetry constraints stemming from the Pauli principle causes additional technical difficulties; in the treatment of the nuclear Schrödinger equation in quantum dynamics, the symmetry constraints are therefore often disregarded, i.e. atoms are treated as distinguishable particles [4].

Unfortunately, besides from the elementary (matrix) case $d=2$, the two classical concepts from tensor product approximation [28], i.e. the canonical or Kronecker decomposition also known as CANDECOMP or PARAFAC, and so-called Tucker decomposition, suffer from different shortcomings. The canonical format, although surely scaling linearly with respect to the order $d$, the dimension $n$ of the vector space and the canonical rank $r$, thus being ideal with regard to complexity, carries a lot of theoretical and practical drawbacks: The set of tensors of fixed canonical rank is not closed, and the existence of a best approximation is not guaranteed [11]. Although in some cases the approximation works quite well [13], optimization methods often fail to converge as a consequence of uncontrollable redundancies in the parametrisation, and an actual computation of a low-rank approximation can thus be a numerically hazardous task. In contrast to this, the Tucker format, in essence corresponding to orthogonal projections into optimal subspaces of $\mathbb{R}^{n}$, still scales exponentially with the order $d$, only reducing the basis from $n$ to the Tucker rank $r$. It thus still suffers from the curse of dimensionality - but provides a stable format from the perspective of practical computations: A quasi-optimal approximation of a given tensor can be computed by higher order SVD (HOSVD) [9]; an optimal approximation of a given tensor can be computed by higher order orthogonal iteration (HOOI, [10]), or by the Newton-Grassmann approach introduced in [12, 40]. Alternatively, usage of alternating least square (ALS) approaches is also recommendable for computation of a best approximation [23, 24, 29].
Most importantly, the Tucker is also well applicable to the discretization of differential equations, e.g. in the context of the MRSCF approach [22] to quantum chemical problems or of multireference Hartree and Hartree-Fock methods (MR-HF) in quantum dynamics.

From a theoretical point of view, the set of Tucker tensors of fixed rank forms an embedded manifold [27], and the numerical treatment therefore follows the general concepts of the numerical treamtent of differential equations on manifolds [20].
On the whole, one is faced with an unsatisfactory situation, confirmed by experiences made through the past decade: On one hand, the canonical format gives an unstable representation of ideal complexity, which cannot be recommended without serious warnings. On the other hand, the stable Tucker format provides the basis for systematic discretization of e.g. inital value problems, but still carries the curse of dimensionality. Recent developments in the field of tensor approximation now seem to offer a way out of this dilemma: Based on the framework of subspace approximation, Hackbusch and Kühn [19] have recently introduced a hierarchical Tucker (HT) format in which only tensors of at most order 3 are used for representation of an order- $d$-tensor. An according decomposition algorithm using hierarchical singular value decompositions and providing a quasi-optimal approximation in the $\ell_{2}$-sense has been introduced by Grasedyck [18]; Hackbusch has also recently shown the existence of a best approximation [15]. Independently, the TT format (abbreviating "tree tensor" or "tensor train"), a special case of the above hierarchical HT structure, was recently introduced by Oseledets and Tyrtyshnikov [34, 38, 39]. This format offers one of the simplest kinds of representation of a tensor in the HT format, and although we conjecture that the results given in this paper can be generalized to the hierarchical tensor format, we will confine ourselves to the particular case of the TT format throughout this work for sake of simplicity.
Without reference to these recent developments, the basic ideas of these new formats format have interestingly enough already been used for the treatment of various problems of many particle quantum physics since almost 20 years, e.g. in quantum dynamics [4], in the computation of finitely correlated states (FCS, [16]) and valence bond solid states (VBS, [25]), in the context of the DMRG algorithm [47], and under the name of matrix product states (MPS, [46]) utilized in the description of spin systems in quantum information theory [42]. A generalization of these ideas are the so-called tensor networks [45], and although the viewpoints on the problems generally posed and solved in physics may be quite different, we think that it is not only of historical interest to mention and utilize the intimate relationship between those developments in different communities.

With this paper, we wish to make a contribution to the approximation of solutions of high-dimensional problems by TT tensors of fixed rank $\underline{r}$ (see Section 2 for the definition). After a review of the TT decomposition and the introduction some notation, we
will start in Section 3 by showing that for a tensor $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$, its TT rank (sometimes also termed compression rank) can be uniquely defined in terms of in some sense optimal TT decompositions of $U$ (i.e. decompositions of minimal rank), and equals the so-called separation rank of $U$, see Section 2.5 and Theorem 3.1. We then continue by analysing the set $\mathbb{T}$ of tensors of fixed TT rank $\underline{r}$, forming a nonlinear manifold. For a formulation of algorithms on $\mathbb{T}$, it is helpful to understand the analytical structure of $\mathbb{T}$, in particular that of its tangent space: If we take the approach persued e.g. in [26] for the low rank approximation of solutions of high dimensional differential equations, or as for other manifolds in [27, 33], the original problem is in each iteration step solved on the tangent space $\mathcal{T}_{U} \mathbb{T}$ of $\mathbb{T}$, taken at the current iterate $U$ - an approach which can be viewed as a Galerkin approximation with the approximation space $\mathcal{T}_{U} \mathbb{T}$ depending on the current iterate $U$. Therefore, we show in Section 4 that the tangent space $\mathcal{T}_{U} \mathbb{T}$ of the TT manifold $\mathbb{T}$ of fixed maximal rank $\underline{r}$, taken at some $U \in \mathbb{T}$, can be uniquely represented by introducing gauge conditions similar to those used in [20, 33], see Theorem 4.2. From our result, we also deduce a unique local parametrization of the TT manifold $\mathbb{T}$ in Section 5, Theorem 5.2. Roughly speaking, our main result states that the manifold of TT format locally provides an embedded manifold, therefore preserving the essential properties of the Tucker format with a complexity scaling linearly with respect to $n$ and $d$, but only quadraticly with respect to the ranks. Section 6 finally uses the results of Section 4 and 5 to exemplify the scope of algorithmic applications of the tangent space $\mathcal{I}_{U} \mathbb{T}$ in the context of approximating solutions of optimization problems and differential equations in high-dimensional spaces.


Figure 1. Examples of graphical representations of tensors, see Section 2.1.

## 2. Review of the TT-Tensor Representation; Notations and definitions

In this section, we will first of all review the basic idea and the various formats used in the different contexts utilizing the TT approximation. As the treatment of tensors naturally involves multi-index quantities, notational matters often tend to make the basic ideas hard to grasp, while they are sometimes conveyed in a clearer way by means of a graphical representation. We will therefore - alongside with the "classical" notation - use a graphical notation inspired by [45] and similar approaches in quantum chemistry, see e.g. [8, 43], and this notation will also be introduced in this section.
2.1. General notes; graphical representation. In the present paper, we are dealing with the representation or approximation of tensors $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ by tensors given in the TT tensor format. In this, the order (or dimension) $d \in \mathbb{N}$ as well as $n_{1}, \ldots, n_{d}$, determining finite index sets $\mathcal{I}_{i}:=\left\{1, \ldots, n_{i}\right\}$ for all $i \in\{1, \ldots, d\}$, will be fixed in the following. For convenience of exposition, we will only treat real-valued tensors here. We will often regard a tensor $U$ as a multivariate function depending on $d$ variables $x_{1}, \ldots, x_{d}$, $x_{i} \in \mathcal{I}_{i}$, and write in the form

$$
\begin{equation*}
U: \mathcal{I}_{1} \times \cdots \times \mathcal{I}_{d} \rightarrow \mathbb{R}, \quad \underline{x}=\left(x_{1}, \ldots, x_{d}\right) \mapsto U\left(x_{1}, \ldots, x_{d}\right) . \tag{2.1}
\end{equation*}
$$

If not prone to arouse confusion, we will sometimes denote $U: \underline{x} \mapsto U(\underline{x})$ by $U(\underline{x})$ for sake of brevity.
Using the graph notation introduced in [45], a tensor $U$ of the above form (2.1) is represented by a dot with $d$ "arms", depicting the $d$ free variables $x_{1}, \ldots, x_{d}$. For example, a tensor (2.1) for which $d=5$ can be symbolized as in Figure 1 (a). Picture (b) and (c) illustrate the special cases $d=1$ and $d=2$, i.e. that of a vector $\mathbf{x} \in \mathbb{R}^{n_{1}}$ and a matrix $\mathbf{A} \in \mathbb{R}^{n_{1} \times n_{2}}$, respectively. Many operations of multilinear algebra involve summations over one or more of the indices (or variables) $x_{i}=1, \ldots, n_{i}$, and such summations are conveniently depicted in the graph representation by joining the respective "arms" of the involved tensors. Thus, a matrix-vector multiplication looks as in (d), yielding again an one-index quantity corresponding to one "free arm", while an SVD may depicted as in (e), with the white two-armed dots representing orthogonal matrices. A globalisation of the SVD is the so-called Tucker decomposition [44] as depicted in (f).
2.2. The TT format. A representation of a tensor $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ in the TT tensor format rewrites an order- $d$ tensor of the form (2.1) as a suitable product of two matrices and $d-2$ tensors of order 3 : Each order- $d$-tensor $U$ of the form (2.1) can be decomposed
into a TT tensor, so that $U(\underline{x})=U\left(x_{1}, \ldots, x_{d}\right)$ can be written as

$$
\begin{equation*}
U(\underline{x})=\sum_{k_{1}=1}^{r_{1}} \ldots \sum_{k_{d-1}=1}^{r_{d-1}} U_{1}\left(x_{1}, k_{1}\right)\left(\prod_{\mu=2}^{d-1} U_{\mu}\left(k_{\mu-1} x_{\mu}, k_{\mu}\right)\right) U_{d}\left(k_{d-1}, x_{d}\right), \tag{2.2}
\end{equation*}
$$

where for $2 \leq i \leq d-1, U_{i} \in \mathbb{R}^{n_{i-1} \times n_{i} \times r_{i}}$,

$$
U_{i}:\left(k_{i-1}, x_{i}, k_{i}\right) \mapsto U_{i}\left(k_{i-1}, x_{i}, k_{i}\right) \in \mathbb{R}^{r_{i-1} \times n_{i} \times r_{i}}
$$

is a tensor of order 3, and matrices

$$
\begin{aligned}
& U_{1}:\left(x_{1}, k_{1}\right) \mapsto U_{1}\left(x_{1}, k_{1}\right) \in \mathbb{R}^{n_{1} \times r_{1}} \\
& U_{d}:\left(k_{d-1}, x_{d}\right) \mapsto U_{d}\left(k_{d-1}, x_{d}\right) \in \mathbb{R}^{r_{d-1} \times n_{d}}
\end{aligned}
$$

form the "ends" of the TT tensor. The numbers $r_{i}$ are the so-called compression ranks, determining the sparsity of the representation (2.2). The (probably more accessible) graphical representation of the TT tensor (2.2) is given in Figure 1(g).
Note that auxiliary variables $k_{i}, i=1, \ldots, d-1$ have been introduced, "connecting" the single components $U_{i}\left(k_{i-1}, x_{i}, k_{i}\right)$ depending on solely one of the old variables $x_{i}$. By the above TT decomposition, the storage requirements can usually be reduced dramatically, e.g. from $n^{d}$ to no more than $r_{\text {max }}^{2} n d$, where $r_{\text {max }}$ is the maximum over $r_{i}, i=1, \ldots, d-1$. A decomposition of $U$ of the form (2.2) can for instance be computed by successive singular value decompositions, see [34] or Section (3.2). Note also that a decomposition of $U$ of the form (2.2) is highly non-unique, see the remarks in Section 2.3.
2.3. Component functions and matrix product representation. In (2.2), the matrices $\left[U_{1}\left(x_{1}, k_{1}\right)\right],\left[U_{d}\left(k_{d}, x_{d}\right)\right]$ can be interpreted as vector-valued functions

$$
\begin{array}{ll}
\mathbf{U}_{1}: \mathcal{I}_{1} \rightarrow \mathbb{R}^{r_{1}}, & \mathbf{U}_{1}\left(x_{1}\right):=\left[U_{1}\left(x_{1}, k_{1}\right)\right]_{k_{1}}^{T}, \\
\mathbf{U}_{d}: \mathcal{I}_{d} \rightarrow \mathbb{R}^{r_{d-1}}, & \mathbf{U}_{d}\left(x_{d}\right):=\left[U_{d}\left(k_{d-1}, x_{d}\right)\right]_{k_{d-1}}
\end{array}
$$

respectively. Analogously, for $2 \leq i \leq d-1$, the 3 -d tensors $U_{i}$ can be seen as matrixvalued functions

$$
\begin{equation*}
\mathbf{U}_{i}: \mathcal{I}_{i} \rightarrow \mathbb{R}^{r_{i-1} \times r_{i}}, \quad x_{i} \mapsto \mathbf{U}_{i}\left(x_{i}\right):=\left[U_{i}\left(k_{i-1}, x_{i}, k_{i}\right)\right]_{k_{i-1}, k_{i}} \tag{2.3}
\end{equation*}
$$

We will call these functions the component functions of the TT representation (2.2) of the tensor $U$. The cases $i=1$ and $i=d$ are formally included in the notation (2.3) by letting $r_{0}=1$ and $r_{d}=1$, respectively. We will also from time to time use the sets

$$
\begin{equation*}
C_{i}:=\left\{\mathbf{U}_{i}: \mathcal{I}_{i} \rightarrow \mathbb{R}^{r_{i-1} \times r_{i}}\right\} \tag{2.4}
\end{equation*}
$$

of all $i$-th component functions. The value $U(\underline{x})$ of $U$ at $\underline{x}=\left(x_{1}, \ldots, x_{d}\right) \in \mathcal{I}_{1} \times \ldots \times \mathcal{I}_{d}$ can now conveniently be written in the matrix product representation,

$$
\begin{equation*}
U(\underline{x})=\mathbf{U}_{1}\left(x_{1}\right) \mathbf{U}_{2}\left(x_{2}\right) \cdot \ldots \cdot \mathbf{U}_{d-1}\left(x_{d-1}\right) \mathbf{U}_{d}\left(x_{d}\right), \tag{2.5}
\end{equation*}
$$

and we will rather use the notation (2.5) than that in (2.2) in the following. Note that for fixed $\underline{x}, \mathbf{U}_{1}\left(x_{1}\right) \in \mathbb{R}^{1 \times r_{1}}$ is a row vector and $\mathbf{U}_{d}\left(x_{d}\right) \in \mathbb{R}^{r_{d-1} \times 1}$ is a column vector, so that $U(\underline{x})$ can be evaluated by a repeated computation of matrix-vector products, explaining the terminology. As introduced here, we will use bold-faced letters for all matrices, vectors and matrix- or vector-valued functions throughout this work.
In the representation (2.5) of a tensor $U$, multiplication of the component function $\mathbf{U}_{i}$ from the right with any invertible matrix $\mathbf{A} \in \mathbb{R}^{r_{i} \times r_{i}}$ and simultaneously of $\mathbf{U}_{i+1}$ with $\mathbf{A}^{-1}$ from the left yields a different TT decomposition for $U$, showing that a decomposition of $U$ of the form (2.2) is highly non-unique. In Section 3, we will formulate conditions under which we obtain a certain uniqueness of the TT decomposition of a tensor $U$, see Theorem 3.1.
2.4. Left and right unfoldings. For the treatment of TT tensors due in the following chapters, we will use some terminology concerned with unfoldings of the above component functions, given in the following.
The left unfolding of a component function (2.3) is the matrix obtained by taking the indices $k_{i-1}, x_{i}$ of the tensor $\left(k_{i-1}, x_{i}, k_{i}\right) \mapsto U_{i}\left(k_{i-1}, x_{i}, k_{i}\right)$ as row indices and the indices $k_{i}$ as column indices,

$$
\mathbf{L}\left(\mathbf{U}_{i}\right) \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times r_{i}}, \quad \mathbf{L}\left(\mathbf{U}_{i}\right)\left(\left(k_{i-1}, x_{i}\right), k_{i}\right):=U_{i}\left(k_{i-1}, x_{i}, k_{i}\right)
$$

See also Fig. 2 for an illustration of the quantities $\mathbf{U}_{i}$ and $\mathbf{L}\left(\mathbf{U}_{i}\right)$. The unfolding mapping

$$
\begin{equation*}
\mathbf{L}: \mathbf{U}_{i} \mapsto \mathbf{L}\left(\mathbf{U}_{i}\right) \tag{2.6}
\end{equation*}
$$

defines a linear bijection between $C_{i}$ and $\mathbb{R}^{\left(r_{i-1} n_{i}\right) \times r_{i}}$. We define the left rank of a component function $\mathbf{U}_{i}(\cdot)$ as the rank of the matrix $\mathbf{L}\left(\mathbf{U}_{i}\right) \in \mathbb{R}^{r_{i} \times r_{i}}$, i.e. the number of linearly independent column vectors of its left unfolding.


Figure 2. Illustration of the quantities $\mathbf{U}_{i}, \mathbf{L}\left(\mathbf{U}_{i}\right),\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]_{\mathbf{G}}$.

Analogously to the above, we define the right unfolding $\mathbf{R}\left(\mathbf{U}_{i}\right)$ $\in \mathbb{R}^{r_{i-1} \times\left(n_{i} r_{i}\right)}$ of $\mathbf{U}_{i}$ as the matrix obtained by taking the indices $k_{i-1}$ of $\mathbf{U}_{i}$ as row indices and the indices $x_{i}, k_{i}$ as column indices, and the right rank of $\mathbf{U}_{i}$ as the rank of $\mathbf{R}\left(\mathbf{U}_{i}\right)$. Cf. also Fig. 2 for an illustration of the quantities $\mathbf{U}_{i}$ and $\mathbf{L}\left(\mathbf{U}_{i}\right)$.

### 2.5. TT decompositions of minimal rank, full-rank-condition, TT rank and

 separation rank. Let $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ be an arbitrary tensor. A TT decomposition$$
\begin{equation*}
U(\underline{x})=\mathbf{U}_{1}\left(x_{1}\right) \mathbf{U}_{2}\left(x_{2}\right) \cdot \ldots \cdot \mathbf{U}_{d-1}\left(x_{d-1}\right) \mathbf{U}_{d}\left(x_{d}\right) \tag{2.7}
\end{equation*}
$$

of the tensor $U$ will be called minimal or fulfilling the full-rank-condition if all component functions $\mathbf{U}_{i}$ have full left and right rank, i.e. the rank of the left unfolding of $\mathbf{U}_{i}$ is $r_{i}$ and the rank of the right unfolding of $\mathbf{U}_{i}$ is $r_{i-1}$. For sake of brevity we will sometimes denote the tensor $U$ given pointwise by $(2.7)$ as $U=\mathbf{U}_{1} \cdot \ldots \cdot \mathbf{U}_{d}$. If (2.7) is a given minimal TT decomposition of $U$, consisting of component functions $\mathbf{U}_{i}: \mathcal{I}_{i} \rightarrow \mathbb{R}^{r_{i-1} \times r_{i}}$ having full left rank $r_{i}$ and full right rank $r_{i-1}$, we will call (2.7) a decomposition of TT rank

$$
\begin{equation*}
\underline{r}:=\left(r_{1}, \ldots, r_{d-1}\right) \tag{2.8}
\end{equation*}
$$

of $U$.
Note that a priori, there may be different TT decompositions (2.7) of $U$, having different TT ranks $\underline{r}$, so that the TT rank is a property of a particular decomposition of $U$, not if $U$ itself. In the next section, we will show though that for any minimal TT decomposition of $U$, the TT rank of this minimal decomposition $\underline{r}$ is equal to the separation rank $\underline{s}$ of $U$, defined next - thus, a minimal $\underline{r}$ is uniquely determined for each tensor $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$, and the TT rank of a tensor $U$ will be defined as this minimal $\underline{r}$ in Theorem 3.1.
By

$$
\begin{equation*}
\mathbf{A}_{i}\left(\left(x_{1}, \ldots, x_{i}\right),\left(x_{i+1}, \ldots, x_{d}\right)\right)=U\left(x_{1}, \ldots, x_{i}, x_{i+1}, \ldots, x_{d}\right) \tag{2.9}
\end{equation*}
$$

we denote the $i$-th canonical unfolding (or matrification) of $U$, i.e. the matrix obtained by taking the indices $x_{1}, \ldots, x_{i}$ of $U$ as row indices and the indices $x_{i+1}, \ldots, x_{d}$ as column indices, see e.g. [28] for details. The unfolding or matrification of a tensor is used several times in this paper in different circumstances where indices $x_{i}$ are replaced by other indices $k_{i}$ etc. The $i$-th separation rank $s_{i}$ of $U$ is then defined as the rank of the $i$-th canonical unfolding $\mathbf{A}_{i}$. The vector

$$
\begin{equation*}
\underline{s}:=\left(s_{1}, \ldots, s_{d}\right) \tag{2.10}
\end{equation*}
$$

will be called the separation rank of $U$.
2.6. Orthogonality constraints. We will say that $\mathbf{U}_{i}$ and $\mathbf{W}_{i}$ are mutually left-orthogonal with respect to an inner product induced by some symmetric positive definite matrix $\mathbf{G} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)}$ iff

$$
\begin{equation*}
\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}}:=\left(\mathbf{L}\left(\mathbf{U}_{i}\right)\right)^{T} \mathbf{G} \mathbf{L}\left(\mathbf{W}_{i}\right)=\mathbf{0} \in \mathbb{R}^{r_{i} \times r_{i}} \tag{2.11}
\end{equation*}
$$

i.e. the columns of the left unfoldings of $\mathbf{U}_{i}$ and $\mathbf{W}_{i}$ are mutually orthogonal with respect to the inner product induced by G. See also Fig. 2 for a graphical representation of $\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}}$.
A component function $\mathbf{U}_{i}$ will be called left-orthogonal (with $\mathbf{G}=\mathbf{I} \in \mathbb{R}^{r_{i-1} n_{i} \times r_{i-1} n_{i}}$ ) iff

$$
\begin{equation*}
\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]:=\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]_{\mathbf{I}}=\mathbf{I} \in \mathbb{R}^{r_{i} \times r_{i}} \tag{2.12}
\end{equation*}
$$

holds, i.e. if the columns of $\mathbf{L}\left(\mathbf{U}_{i}\right)$ are an orthonormal system. In the same way we define that $\mathbf{U}_{i}$ is right-orthogonal iff

$$
\begin{equation*}
\mathbf{R}\left(\mathbf{U}_{i}\right)\left(\mathbf{R}\left(\mathbf{U}_{i}\right)\right)^{T}=\mathbf{I} \in \mathbb{R}^{r_{i-1} \times r_{i-1}} \tag{2.13}
\end{equation*}
$$

holds.
Without going into much detail, we note that a tensor may be represented in various TT formats being special cases or equivalent representations of (2.5). For example, the canonical proceeding of SVD from left to right gives a tensor with the components $\mathbf{U}_{i}$ being left-orthogonal for $i=1, \ldots, d$, as depicted in Fig. 3(a), where the dots being white at the arms belonging to the indices $k_{i-1}, x_{i}$ indicate left-orthogonality. More globally, one can pick $i \in\{1, \ldots, d\}$ and decompose $U$ by SVDs from the left and the right into a TT tensor the components of which are left-orthogonal for $j<i$ and right-orthogonal for $j>i$, cf. (b). Subsequent QR-decomposition of $\mathbf{U}_{i}$ yields another equivalent representation with invertible $D$, as given in (c). The index $i$ chosen above may even vary during some algorithmic applications, as is for instance the case in the intermediate stages of the DMRG algorithm used in quantum physics (cf. [47]).


## 3. Uniqueness statements for the TT Rank $\underline{r}$ and for TT decompositions

In this section, we prove the following theorem. Part (a) is an extension of results from the two publications [34, 35], where existence of TT decompositions with TT ranks $r_{i} \leq s_{i}$ and $r_{i}=s_{i}$, respectively, is proven. It shows that for of each minimal TT decomposition, its TT rank coincides with the separation rank and thus is a uniquely defined quantity for each tensor $U$. In (b), we then give a certain uniqueness statement for TT decompositions of minimal rank of a tensor $U$. Part (c) shows that in practice, a minimal rank TT decomposition can be computed by successive SVDs, i.e. by the algorithm proposed by Oseledets in [36].

Theorem 3.1. (Uniqueness of TT decompositions; the TT rank of a tensor) Let $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ an arbitrary tensor.
(a) There is exactly one rank vector $\underline{r}$ such that $U$ admits for a TT decomposition

$$
U: \underline{x} \mapsto U(\underline{x})=\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right),
$$

of minimal rank $\underline{r}$. If $\underline{s}=\underline{s}(U)$ denotes the (unique) separation rank of $U$, there holds

$$
\begin{equation*}
\underline{r}=\underline{s} \tag{3.1}
\end{equation*}
$$

Therefore, the separation rank $\underline{r}=\underline{s}$ will also be called the TT rank of the tensor $U$.
(b) The TT decomposition (3.1) of $U$ of minimal rank can be chosen such that the component functions are left-orthogonal,

$$
\begin{equation*}
\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]=\mathbf{I} \in \mathbb{R}^{r_{i} \times r_{i}} \tag{3.2}
\end{equation*}
$$

for all $i=1, \ldots, d-1$ (see [34] for the constructive proof). Under this condition, the decomposition (3.1) is unique up to insertion of orthogonal matrices: For any two left-orthogonal minimal decompositions of $U$ (for which

$$
\begin{equation*}
U(\underline{x})=\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)=\mathbf{V}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{V}_{d}\left(x_{d}\right) \tag{3.3}
\end{equation*}
$$

holds for all $\left.\underline{x}=\left(x_{1}, \ldots, x_{d}\right) \in \mathcal{I}_{1} \times \ldots \times \mathcal{I}_{d}\right)$, there exist orthogonal $\mathbf{Q}_{1}, \ldots, \mathbf{Q}_{d-1}$, $\mathbf{Q}_{i} \in \mathbb{R}^{r_{i} \times r_{i}}$ such that

$$
\begin{gather*}
\mathbf{U}_{1}\left(x_{1}\right) \mathbf{Q}_{1}=\mathbf{V}_{1}\left(x_{1}\right), \quad \mathbf{Q}_{d-1}^{T} \mathbf{U}_{d}\left(x_{d}\right)=\mathbf{V}_{d}\left(x_{d}\right), \\
\mathbf{Q}_{i-1}^{T} \mathbf{U}_{i}\left(x_{i}\right) \mathbf{Q}_{i}=\mathbf{V}_{i}\left(x_{i}\right) \quad \text { for } \quad i=2, \ldots, d-1, \quad \underline{x} \in \mathcal{I}_{1} \times \ldots \times \mathcal{I}_{d} \tag{3.4}
\end{gather*}
$$

(c) Let $U \neq 0$. In Figure 4, we reproduced the SVD-based TT decomposition algorithm introduced in Oseledets [34]. This algorithm, when applied to $U$ without truncation steps and in exact arithmetic, returns a minimal TT decomposition with left-orthogonal component functions $\mathbf{U}_{i}$ (see (3.2)).

Remark 3.2. Theorem 3.1 uniquely defines a minimal TT rank $\underline{r}$ for any tensor $U$. This rank $\underline{r}$ is attained by any TT decomposition of $U$ fulfilling the full-rank -condition (see Sec. 2.5). Note that $\underline{r}$ is not invariant under permutations of indices (because the separation rank is not). In particular, the arrangement of indices might influence the complexity of the storage needed to represent $U$ in the TT format.
Also, Theorem 3.1 implies a new (without further information sharp) bound on the TT rank of a tensor $U$ : Because

$$
\begin{equation*}
m_{i}:=\min \left\{\prod_{j=1}^{i} n_{j}, \prod_{j=i+1}^{d} n_{j}\right\} \tag{3.5}
\end{equation*}
$$

defines the maximal rank possible for an SVD of the $i$-th canonical unfolding, Theorem 3.1 shows

$$
\begin{equation*}
r_{i} \leq m_{i} \tag{3.6}
\end{equation*}
$$

Figure 4. The successive SVD-algorithm for computing a TT decomposition.
Input: $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}} ; \quad$ Output: $\mathbf{U}_{i} \in C_{i}, i=1, \ldots, d$.
Set $\mathbf{B}_{(1)}=\mathbf{A}_{1}$ ( $\mathbf{A}_{1}$ is the first canonical unfolding)
Set $r_{1}:=\operatorname{rank} \mathbf{B}_{(1)}$
Compute the SVD $\mathbf{B}_{(1)}=\left[\sum_{k_{1}=1}^{r_{1}} \mathbf{U}_{1}\left(x_{1}, k_{1}\right) \mathbf{V}_{(1)}\left(k_{1},\left(x_{2}, \ldots, x_{d}\right)\right)\right]_{x_{1},\left(x_{2}, \ldots, x_{d}\right)}$ with left-orthogonal $\mathbf{U}_{1}$
for $i=2, \ldots, d-1$ do
Set $\mathbf{B}_{(i)}\left(\left(x_{i}, k_{i-1}\right),\left(x_{i+1}, \ldots, x_{d}\right)\right)=\mathbf{V}_{(i-1)}\left(k_{i-1},\left(x_{i}, \ldots, x_{d}\right)\right)$
Set $r_{i}:=\operatorname{rank} \mathbf{B}_{(i)}$
Compute the SVD

$$
\mathbf{B}_{(i)}=\left[\sum_{k_{i}=1}^{r_{i}} \mathbf{U}_{i}\left(\left(x_{i}, k_{i-1}\right), k_{i}\right) \mathbf{V}_{(i)}\left(k_{i},\left(x_{i+1}, \ldots, x_{d}\right)\right)\right]_{\left(x_{i}, k_{i-1}\right),\left(x_{i+1}, \ldots, x_{d}\right)}
$$ with left-orthogonal $\mathbf{U}_{i}$

end for
$\operatorname{Set} \mathbf{U}_{d}\left(x_{d}, k_{d-1}\right):=\mathbf{V}_{(d)}\left(k_{d-1}, x_{d}\right)$
for all $i=1, \ldots, d-1$.
Before we approach the proof of Theorem 3.1, we finally note that the uniqueness statements of Theorem 3.1 hold analogously if for fixed $i \in\{1, \ldots, d\}$, the left-orthogonality conditions (3.2) are replaced by left-orthogonality in the first $j<i$ components and by the according right-orthogonality condition $\mathbf{R}\left(\mathbf{U}_{j}\right)\left(\mathbf{R}\left(\mathbf{U}_{j}\right)\right)^{T}=\mathbf{I}$ for $j>i$, so that tensors are required to be of the form depicted in Fig. 3 (b). Analogous globalisations hold for Theorem 4.2, Theorem 5.2 (with the gauge condition (4.6) modified appropriately).
3.1. Notations for left and right parts of a TT tensor. For the proof of Theorem 3.1 and also in the later chapters, we will need some more formal notation concerned with certain unfoldings of parts of $U$, and they are introduced in the following.
For $i \in\{1, \ldots, d\}$ we define the $i$-th left part

$$
\begin{equation*}
\mathbf{U}^{\leq i}=\left[\mathbf{U}^{\leq i}\left(\left(x_{1}, \ldots, x_{i}\right), k_{i}\right)\right]_{\left(x_{1}, \ldots, x_{i}\right), k_{i}} \in \mathbb{R}^{\left(n_{1} \cdots \cdot n_{i}\right) \times r_{i}} \tag{3.7}
\end{equation*}
$$

as the unfolding of the tensor $\left(\mathbf{U}_{1} \cdots \mathbf{U}_{i}\right) \in \mathbb{R}^{n_{1} \times \ldots \times n_{i} \times r_{i}}$ given pointwise by

$$
\begin{equation*}
\left[\mathbf{U}_{1} \cdots \mathbf{U}_{i}\right]_{x_{1}, \ldots, x_{i}, k_{i}}:=\sum_{k_{1}=1}^{r_{1}} \ldots \sum_{k_{i-1}=1}^{r_{i-1}} U_{1}\left(x_{1}, k_{1}\right) \prod_{\mu=2}^{i} U_{\mu}\left(k_{\mu-1}, x_{\mu}, k_{\mu}\right) \tag{3.8}
\end{equation*}
$$

obtained by taking $x_{1}, \ldots, x_{i}$ as row indices and $k_{i}$ as column index. Analogously, the $i$-th right part

$$
\mathbf{U}^{\geq i}=\left[\mathbf{U}^{\geq i}\left(k_{i-1},\left(x_{i}, \ldots, x_{d}\right)\right)\right]_{k_{i-1},\left(x_{i}, \ldots, x_{d}\right)} \in \mathbb{R}^{r_{i-1} \times\left(n_{i} \cdots \cdot n_{d}\right)}
$$

of $U$ is the unfolding of the tensor $\left(\mathbf{U}_{i} \cdots \mathbf{U}_{d}\right) \in \mathbb{R}^{r_{i-1} \times n_{i} \times \ldots \times n_{d}}$ given pointwise by

$$
\left[\mathbf{U}_{i} \cdots \mathbf{U}_{d}\right]_{k_{i-1}, x_{i}, \ldots, x_{d}}:=\sum_{k_{i}=1}^{r_{i}} \ldots \sum_{k_{d-1}=1}^{r_{d-1}}\left(\prod_{\mu=i}^{d-1} U_{\mu}\left(k_{\mu-1}, x_{\mu}, k_{\mu}\right)\right) U_{d}\left(x_{d}, k_{d-1}\right)
$$

taking $x_{i}, \ldots, x_{d}$ as column indices and $k_{i}$ as row index. For formal reasons, we additionally define $\mathbf{U}^{\leq 0}:=(1)=: \mathbf{U}^{\geq d+1}$. Note that $\mathbf{U}^{\leq d}$ and $\mathbf{U}^{\geq d}$ yield a vectorization of the tensor $U$ as a column vector and as a row vector, respectively.
For two given TT representations of tensors $U, V$ and $i \in\{0, \ldots, d\}$, we define the $i$-th left half product matrix $\llbracket U, V \rrbracket^{\leq i}:=\left(\mathbf{U}^{\leq i}\right)^{T} \mathbf{V}^{\leq i} \in \mathbb{R}^{r_{i} \times r_{i}}$ by

$$
\begin{equation*}
\llbracket U, V \rrbracket^{\leq i}\left(k_{i}, k_{i}^{\prime}\right)=\sum_{x_{1}=1}^{n_{1}} \ldots \sum_{x_{i}=1}^{n_{i}} \mathbf{U}^{\leq i}\left(\left(x_{1}, \ldots, x_{i}\right), k_{i}\right) \mathbf{V}^{\leq i}\left(\left(x_{1}, \ldots, x_{i}\right), k_{i}^{\prime}\right) \tag{3.9}
\end{equation*}
$$

for $k_{i}, k_{i}^{\prime} \in\left\{1, \ldots, r_{i}\right\}$.

For formal reasons, we additionally define $\mathbf{U}^{\leq 0}:=1=: \mathbf{U}^{\geq d+1}$. Note that $\mathbf{U}^{\leq d}$ and $\mathbf{U}^{\geq d}$ yield a vectorization of the tensor $U$ as a column vector and as a row vector, respectively.

Analogously, we introduce for $i \in\{1, \ldots, d+1\}$ the $i$-th right half product matrix,

$$
\llbracket U, V \rrbracket^{\geq i}:=\mathbf{U}^{\geq i}\left(\mathbf{V}^{\geq i}\right)^{T} \in \mathbb{R}^{r_{i-1} \times r_{i-1}} .
$$

Fig. 5 (a), (b) illustrate the quantities $\mathbf{U} \leq i$ and $\llbracket U, V \rrbracket^{\leq i}$.
The following recursive formula will play a central role later: For $i \in\{1, \ldots, d\}$, there holds with $G_{i}:=\llbracket U, U \rrbracket^{\leq i-1} \otimes \mathbf{I}_{n_{i} \times n_{i}}$

$$
\begin{align*}
& \llbracket U, U \rrbracket^{\leq i}\left(k_{i}, k_{i}^{\prime}\right)=\left[\mathbf{L}\left(\mathbf{U}_{i}\right)^{T}\left(\llbracket U, U \rrbracket^{\leq i-1} \otimes \mathbf{I}_{n_{i} \times n_{i}}\right) \mathbf{L}\left(\mathbf{U}_{i}\right)\right]_{k_{i}, k_{i}^{\prime}} \\
= & \sum_{k_{i-1}=1}^{r_{i-1}} \sum_{k_{i-1}^{\prime}=1}^{r_{i-1}} \sum_{x_{i}^{\prime}=1}^{n_{i}} \sum_{x_{i}^{\prime}=1}^{n_{i}} G_{i}\left(k_{i}, x_{i}, k_{i}^{\prime}, x_{i}^{\prime}\right) U_{i}\left(k_{i-1}, x_{i}, k_{i}\right) U_{i}\left(k_{i-1}^{\prime}, x_{i}^{\prime}, k_{i}^{\prime}\right) . \tag{3.10}
\end{align*}
$$

where for two matrices $A, B, A \otimes B$ denotes the Kronecker product of $A$ and $B$ here and in the following.
(a)

(b)

(c)


Figure 5. (a) Illustration of $U^{\leq i}$. (b),(c) Two ways to obtain $\llbracket U, V \rrbracket^{\leq i}$.
3.2. Proof of Theorem 3.1(a). We start the proof of Theorem 3.1(a) by showing the existence of a TT decomposition of minimal rank. First of all, we note that the zero tensor $0 \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ can be written as an elementary tensor built up from the zero vectors $0^{(i)} \in \mathbb{R}^{n_{i}}$, giving a minimal TT decomposition for 0 . We now show that for a non-trivial tensor $U \neq 0$, a TT representation of minimal rank can be computed by the algorithm given in Fig. 4.

Lemma 3.3. For a given non-trivial tensor $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$, the algorithm in Fig. 4 returns (in exact arithmetic) a TT decomposition $\left(\mathbf{U}_{1}, \ldots, \mathbf{U}_{d}\right) \in C_{1} \times \ldots \times C_{d}$ with full
left and right rank for each component function $\mathbf{U}_{i}, i=1, \ldots, d$.
Also, the component funtions $\mathbf{U}_{i}, i=1, \ldots, d-1$ are left-orthogonal.
Proof. From the properties of the SVD, it is clear that the algorithm gives back a representation with full left rank and left-orthogonal component functions $\mathbf{U}_{1}, \ldots, \mathbf{U}_{d-1}$. Assume that for some $i \in\{1, \ldots, d\}$, a component function $\mathbf{U}_{i}$ is without full right rank. If $i=1$, $U$ is the zero tensor in contradiction to the assumption that $U$ is non-trivial. If we have $\hat{r}:=\operatorname{rank} \mathbf{R}\left(\mathbf{U}_{i}\right)<r_{i-1}$ for $i>1$, an SVD of $\mathbf{R}\left(\mathbf{U}_{i}\right)$ yields

$$
\mathbf{R}\left(\mathbf{U}_{i}\right)=\mathbf{V} \mathbf{W}, \quad \mathbf{V} \in \mathbb{R}^{r_{i-1} \times \hat{r}}, \quad \mathbf{W} \in \mathbb{R}^{\hat{r} \times n_{i} r_{i}} .
$$

Setting $\widehat{\mathbf{U}}_{i-1}:=\mathbf{L}^{-1}\left(\mathbf{L}\left(\mathbf{U}_{i-1}\right) \mathbf{V}\right)$ and $\widehat{\mathbf{U}}_{i}:=\mathbf{R}^{-1}(\mathbf{W})$, there holds

$$
\widehat{\mathbf{U}}_{i-1}\left(x_{i-1}\right) \widehat{\mathbf{U}}_{i}\left(x_{i}\right)=\mathbf{U}_{i-1}\left(x_{i-1}\right) \mathbf{U}_{i}\left(x_{i}\right) .
$$

For the unfolded matrix $\mathbf{B}_{(i-1)}$ from the algorithm in Fig. 4, this implies that

$$
\sum_{\hat{k}=1}^{\hat{r}} \hat{U}_{i-1}\left(k_{i-2}, x_{i-1}, \hat{k}\right)\left(\sum_{k_{i}=1}^{r_{i}} \ldots \sum_{k_{d-1}=1}^{r_{d-1}} \hat{U}_{i}\left(\hat{k}, x_{i}, k_{i}\right) \prod_{\mu=i+1}^{d} U_{\mu}\left(k_{\mu-1}, x_{\mu}, k_{\mu}\right)\right)
$$

represents also a rank- $\hat{r}$-SVD of $\mathbf{B}_{(i-1)}$. Because of the uniqueness of SVD ranks, this would mean that the left rank $r_{i-1}$ of $\mathbf{U}_{i-1}$ equals $\hat{r}$, a contradiction.

The preceding lemma already proves part (c) of Theorem 3.1. For the proof of (a), it remains to show uniqueness of the TT $\operatorname{rank} \underline{r}=\underline{r}(U)$ for a given tensor $U$. The proof bases essentially on the observation (a) in the next lemma. The statement made in (b) will also be used later to prove the central Theorem 4.2 of Section 4.

Lemma 3.4. Let $U \in \mathbb{T}$ be a minimal $T T$-tensor of rank $\underline{r}$.
(a) For all $i \in\{1, \ldots, d-1\}$, the matrices $\mathbf{U}^{\leq i}, \mathbf{U}^{\geq i+1}$ have rank $r_{i}$.
(b) The matrices

$$
\begin{equation*}
\mathbf{G}_{i}:=\llbracket U, U \rrbracket^{\leq i-1} \otimes \mathbf{I}_{n_{i} \times n_{i}} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)} \tag{3.11}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathbf{P}_{i}:=\llbracket U, U \rrbracket \geq i \in \mathbb{R}^{r_{i-1} \times r_{i-1}} \tag{3.12}
\end{equation*}
$$

are symmetric and positive definite for all $i \in\{1, \ldots, d\}$.

Proof. If $U \in \mathbb{T}$ is a minimal TT-tensor, the component functions $\mathbf{U}_{i}$ have full left and right ranks $r_{i}$ resp. $r_{i-1}$ for all $1 \leq i \leq d$. We only show that if $\mathbf{U}_{j}$ has full left rank for all $1 \leq j<i$ (i.e. $\mathbf{L}\left(\mathbf{U}_{j}\right)^{T} \mathbf{L}\left(\mathbf{U}_{j}\right)$ has full rank $\left.r_{j}\right)$, then $\llbracket U, U \rrbracket^{\leq i-1}:=\left(\mathbf{U}^{\leq i-1}\right)^{T} \mathbf{U}^{\leq i-1}$ and $\mathbf{G}_{i}$ are positive definite; in particular, we then obtain that $\mathbf{U}^{\leq i}$ has full rank $r_{i}$ for all $1 \leq i \leq d-1$. An analogous argument applies to $\mathbf{R}\left(\mathbf{U}_{i}\right)\left(\mathbf{R}\left(\mathbf{U}_{i}\right)\right)^{T}$, finishing the proof. We proceed by induction. For $i=1, \llbracket U, U \rrbracket^{\leq 0}=(1)$ and $\mathbf{G}_{1}$ are positive definite. For the induction step, let the hypothesis hold for $\left(\mathbf{U}^{\leq i-1}\right)^{T} \mathbf{U}^{\leq i-1}$ and $\mathbf{G}_{i}$, and let $\mathbf{L}\left(\mathbf{U}_{i}\right)^{T} \mathbf{L}\left(\mathbf{U}_{i}\right)$ have full rank. Then, the columns of $\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)$ are linearly independent. This means that the Gramian matrix $\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)^{T}\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)$ is positive definite, i.e. there holds

$$
\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)^{T}\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)>0
$$

Using the recursion formula (3.10), $\llbracket U, U \rrbracket \leq i$ can be rewritten inductively as

$$
\begin{aligned}
\llbracket U, U \rrbracket^{\leq i} & =\mathbf{L}\left(\mathbf{U}_{i}\right)^{T}(\llbracket U, U \rrbracket \leq i-1 \\
& =\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)^{T}\left(\mathbf{G}_{i}^{1 / 2} \mathbf{L}\left(\mathbf{U}_{i}\right)\right)>0
\end{aligned}
$$

which also implies that $\mathbf{G}_{i+1}:=\llbracket U, U \rrbracket^{\leq i} \otimes \mathbf{I}_{n_{i+1} \times n_{i+1}}>0$ holds, completing the proof.
We are now in the position to show that for any minimal TT decomposition, its TT rank is equal to the separation rank of $U$ : The $i$-th canonical unfolding $\mathbf{A}_{i}$ of $U$ can be written as the matrix product

$$
\mathbf{A}_{i}=\mathbf{U}^{\leq i} \mathbf{U}^{\geq i+1}
$$

of the $i$-th left part and the $(i+1)$-th right part of $U$, both having full rank $r_{i}$ according to Lemma 3.4(a). We use the $Q R$-decompositions

$$
\mathbf{U}^{\leq i}=\mathbf{Q}_{i} \mathbf{S}_{i}, \quad\left(\mathbf{U}^{\geq i+1}\right)^{T}=\mathbf{Q}_{i+1}^{\prime} \mathbf{S}_{i+1}^{\prime},
$$

where $\mathbf{S}_{i}, \mathbf{S}_{i+1}^{\prime} \in \mathbb{R}^{r_{i} \times r_{i}}$ have full rank $r_{i}$, to obtain

$$
\begin{equation*}
\mathbf{A}_{i}=\mathbf{Q}_{i} \mathbf{S}_{i}\left(\mathbf{S}_{i+1}^{\prime}\right)^{T}\left(\mathbf{Q}_{i+1}^{\prime}\right)^{T}=: \mathbf{Q}_{i} \mathbf{S}\left(\mathbf{Q}_{i+1}^{\prime}\right)^{T} \tag{3.13}
\end{equation*}
$$

with $\mathbf{Q}_{i}, \mathbf{Q}_{i+1}^{\prime}$ having orthonormal columns, and $\mathbf{S}$ having full rank $r_{i}$. Diagonalization of the right hand side of (3.13) yields an SVD of $A_{i}$; thus

$$
s_{i}=\operatorname{rank} \quad \mathbf{A}_{i}=r_{i} .
$$

3.3. Proof of Theorem 3.1 (b). The proof of part (b) uses the following simple lemma.

Lemma 3.5. Let $\mathbf{M}_{1}, \mathbf{N}_{1} \in \mathbb{R}^{p \times r}, \mathbf{M}_{2}, \mathbf{N}_{2} \in \mathbb{R}^{r \times q}$ matrices of rankr. If

$$
\begin{equation*}
\mathbf{M}_{1} \mathbf{M}_{2}=\mathbf{N}_{1} \mathbf{N}_{2} \quad \text { and } \quad \mathbf{M}_{1}^{T} \mathbf{M}_{1}=\mathbf{N}_{1}^{T} \mathbf{N}_{1}=\mathbf{I} \in \mathbb{R}^{r \times r} \tag{3.14}
\end{equation*}
$$

there is an orthogonal matrix $\mathbf{Q}$ such that

$$
\begin{equation*}
\mathbf{M}_{1}=\mathbf{N}_{1} \mathbf{Q}, \quad \mathbf{M}_{2}=\mathbf{Q}^{T} \mathbf{N}_{2} \tag{3.15}
\end{equation*}
$$

Proof. There holds $\mathbf{M}_{2}=\mathbf{M}_{1}^{T} \mathbf{N}_{1} \mathbf{N}_{2}$ and therefore

$$
\begin{aligned}
\mathbf{N}_{2} & =\mathbf{N}_{1}^{T} \mathbf{N}_{1} \mathbf{N}_{2}=\mathbf{N}_{1}^{T} \mathbf{M}_{1} \mathbf{M}_{2}=\mathbf{N}_{1}^{T} \mathbf{M}_{1} \mathbf{M}_{1}^{T} \mathbf{N}_{1} \mathbf{N}_{2} \\
& =\mathbf{N}_{1}^{T} \mathbf{M}_{1}\left(\mathbf{N}_{1}^{T} \mathbf{M}_{1}\right)^{T} \mathbf{N}_{2}
\end{aligned}
$$

This implies that $\mathbf{Q}:=\mathbf{N}_{1}^{T} \mathbf{M}_{1} \in \mathbb{R}^{r \times r}$ is an orthogonal matrix because the columns of $\mathbf{N}_{2}$ span $\mathbb{R}^{r}$. Using $\mathbf{M}_{2}=\mathbf{M}_{1}^{T} \mathbf{N}_{1} \mathbf{N}_{2}$ again yields $\mathbf{M}_{2}=\mathbf{Q}^{T} \mathbf{N}_{2}$ and also

$$
\mathbf{N}_{1} \mathbf{N}_{2}=\mathbf{M}_{1} \mathbf{M}_{2}=\mathbf{M}_{1} \mathbf{Q}^{T} \mathbf{N}_{2}
$$

which implies $\mathbf{M}_{1} \mathbf{Q}^{T}=\mathbf{N}_{1}$ due to the full rank of $\mathbf{N}_{2}$.
The assertion of Theorem part (b) now follows by inductively applying the result of the Lemma 3.5 to the sequence of matrices $\left(\mathbf{Q}_{i-1}^{T} \otimes \mathbf{I}\right) \mathbf{L}\left(\mathbf{U}_{i}\right) \in \mathbb{R}^{r_{i-1} \cdot n_{i} \times r_{i}}, \mathbf{U}^{\geq i+1} \in$ $\mathbb{R}^{r_{i} \times\left(n_{i+1} \cdots \cdot n_{d}\right)}$ formed from the component functions $\mathbf{U}_{i}$ belonging to the left representation of $U$ in (3.3) (where $\mathbf{Q}_{0}=(1)$ ), and to $\mathbf{V}_{i}, \mathbf{V}^{\geq i+1}$ analogously formed from the right hand representation: We at first note that Lemma 3.4(a) ensures that these matrices have rank $r_{i}$. Further, if $\mathbf{Q}_{i-1}$ is orthogonal, $\mathbf{Q}_{i-1} \otimes \mathbf{I}$ is orthogonal. Thus, the conditions (3.14) of Lemma 3.5 are satisfied. If (3.3) holds, we thus get inductively that

$$
\begin{gathered}
\mathbf{L}\left(\mathbf{U}_{1}\right)=\mathbf{L}\left(\mathbf{V}_{1}\right) \mathbf{Q}_{1}, \quad \mathbf{L}\left(\mathbf{U}_{i}\right)=\left(\mathbf{Q}_{i-1}^{T} \otimes \mathbf{I}\right) \mathbf{L}\left(\mathbf{V}_{i}\right) \mathbf{Q}_{i} \\
\mathbf{U}^{\geq 2}=\left[\mathbf{U}_{2}(\cdot) \cdot \ldots \cdot \mathbf{U}_{d}(\cdot)\right]=\left[\left(\mathbf{Q}_{1}^{T} \mathbf{V}_{2}(\cdot)\right) \cdot \mathbf{V}_{3}(\cdot) \cdot \ldots \cdot \mathbf{V}(\cdot)_{d}\right] ; \\
\mathbf{U}^{\geq i+1}=\left[\mathbf{U}_{i+1}(\cdot) \cdot \ldots \cdot \mathbf{U}_{d}(\cdot)\right]=\left[\left(\mathbf{Q}_{i}^{T} \mathbf{V}_{i+1}(\cdot)\right) \mathbf{V}_{i+2}(\cdot) \cdot \ldots \cdot \mathbf{V}_{d}(\cdot)\right]
\end{gathered}
$$

which proves the assertion by the observation that

$$
\begin{aligned}
\mathbf{L}\left(\mathbf{U}_{i}\right)=\left(\mathbf{Q}_{i-1}^{T} \otimes \mathbf{I}\right) \mathbf{L}\left(\mathbf{V}_{i}\right) \mathbf{Q}_{i} \quad \Longleftrightarrow \quad & \mathbf{U}_{i}\left(x_{i}\right)=\mathbf{Q}_{i-1}^{T} \mathbf{V}_{i}\left(x_{i}\right) \mathbf{Q}_{i} \\
& \text { for all } x_{i} \in\left\{1, \ldots, n_{i}\right\}
\end{aligned}
$$

In the final step $i=d-1$, we obtain $\mathbf{U}^{\geq d}=\mathbf{R}\left(\mathbf{U}_{d}\right)=\mathbf{Q}_{d-1}^{T} \mathbf{R}\left(\mathbf{V}_{d}\right)$, finishing the proof.

## 4. The manifold of TEnsors of fixed TT RANK And its TANGENT space

4.1. The manifold of tensors of fixed TT rank $\underline{r}$. From this point on, we will be concerned with the manifold $\mathbb{T}_{\underline{r}}$ formed by the $d$-dimensional TT tensors $U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ of fixed rank $\underline{r}=\left(r_{1}, \ldots, r_{d}\right)$,

$$
\begin{equation*}
\mathbb{T}:=\mathbb{T}_{\underline{r}}:=\left\{U \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}} \text { is tensor of TT rank } \underline{r}\right\} \tag{4.1}
\end{equation*}
$$

Theorem 3.1 implies that $\mathbb{R}^{n_{1} \times \ldots n_{d}}$ is the disjoint union of the manifolds $\mathbb{T}_{\underline{r}}$, with the possible values of $\underline{r}$ restricted by (3.5).

Before we mainly turn our attention to the tangent space of $\mathbb{T}$ in the subsequent sections, we make the following observation:

Lemma 4.1. Let a rank vector $\underline{r}=\left(r_{1}, \ldots, r_{d-1}\right)$ be given, $r_{0}=r_{d}=1$ as before. For fixed $d, n_{1}, \ldots, n_{d} \in \mathbb{N}, \mathbb{T}_{\underline{r}}$ is a manifold of dimension

$$
\begin{equation*}
\operatorname{dim} \mathbb{T}=\sum_{i=1}^{d} r_{i-1} n_{i} r_{i}-\sum_{i=1}^{d-1} r_{i}^{2} \tag{4.2}
\end{equation*}
$$

Proof. The assertion follows from Theorem 3.1: Let us define

$$
f: \times_{i=1}^{d} C_{i} \rightarrow \mathbb{R}^{n_{1} \times \ldots \times n_{d}},
$$

given by

$$
\left(x_{1} \mapsto \mathbf{U}_{1}\left(x_{1}\right), \ldots, x_{d} \mapsto \mathbf{U}_{d}\left(x_{d}\right)\right) \mapsto\left(\left(x_{1}, \ldots, x_{d}\right) \mapsto \mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)\right)
$$

and an equivalence relation $\sim$ on $\times{ }_{i=1}^{d} C_{i}$ by

$$
\begin{aligned}
& \left(\mathbf{U}_{1}(\cdot), \ldots, \mathbf{U}_{d}(\cdot)\right) \sim\left(\mathbf{V}_{1}(\cdot), \ldots, \mathbf{V}_{d}(\cdot)\right) \\
\Longleftrightarrow \quad & (3.4) \text { holds for some orthogonal } \mathbf{Q}_{i} \in \mathbb{R}^{r_{i} \times r_{i}}, i=1, \ldots, d .
\end{aligned}
$$

Note that $f$ is also well defined on the factorized space $\mathcal{V}:=\times_{i=1}^{d} C_{i} / \sim$ (by application to arbitrary representants). Let us define an auxiliary manifold $\mathcal{M} \subseteq \mathcal{V}$ by the constraint conditions

$$
\begin{equation*}
g_{i}\left(\mathbf{U}_{1}, \ldots, \mathbf{U}_{d}\right):=\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]=\mathbf{I} \in \mathbb{R}^{r_{i} \times r_{i}}, \quad i=1, \ldots, d-1 \tag{4.3}
\end{equation*}
$$

The set GL $\left(r_{i} \times r_{i}\right)$ of invertible matrices $A \in \mathbb{R}^{r_{i} \times r_{i}}$ is open and the mappings $\mathbf{U}_{i} \mapsto\left[\mathbf{U}_{i}, \mathbf{U}_{i}\right]$, $\mathbf{U}_{i} \mapsto \mathbf{R}\left(\mathbf{U}_{i}\right)^{T} \mathbf{R}\left(\mathbf{U}_{i}\right)$ are continuous; thus, for any $\left(\mathbf{U}_{1}, \ldots, \mathbf{U}_{d}\right)$ for which the $\mathbf{U}_{i}$ have full left and right rank, there is a neighbourhood $N_{\delta}$ such that for $\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right) \in N_{\delta}$, each $\mathbf{W}_{i}$ still has full left and right rank. For $D:=\mathcal{M} \cap N_{\delta}$,
the restriction $\left.f\right|_{D}: D \rightarrow f(D)$ therefore maps to $\mathbb{T}$. Obviously, $\left.f\right|_{D}$ is continuous, and bijective by Theorem 3.1. Thus, a further restriction of $\left.f\right|_{D}$ to a compact subset $K$ of $D$ with nonempty interior possesses a continuous inverse. Yet another restriction $\left.f\right|_{L}$ to an open subset $L \subseteq K$ containing $U$ gives a local chart for $\mathbb{T}$ containing $U$, and a suitable collection of such restrictions for all $U \in \mathbb{T}$ thus constitutes an $\mathcal{M}$-atlas [31] of $\mathbb{T}$. Thus, the dimensions of $\mathbb{T}$ and $\mathcal{M}$ coincide. To determine the latter, we first note that orthogonal $\mathbb{R}^{r_{i} \times r_{i}}$-matrices are determined by $r_{i}\left(r_{i}-1\right) / 2$ degrees of freedom, so that the factorization with respect to $\sim$ gives that for $\mathcal{V}$,

$$
\operatorname{dim} \mathcal{V}=\sum_{i=1}^{d} r_{i-1} n_{i} r_{i}-\sum_{i=1}^{d-1} \frac{r_{i}\left(r_{i}-1\right)}{2}
$$

In analogy to the constraint conditions imposed on the Stiefel manifold (see e.g. [20]), it is not hard to see that the constraint (4.3) yields $r_{i}\left(r_{i}+1\right) / 2$ independent constraint conditions in each component, so that the Jacobian of accordingly constructed constraint function $g$ has full rank $\sum_{i=1}^{d-1} r_{i}\left(r_{i}+1\right) / 2$. This implies (see also [20], IV.5.1) that

$$
\operatorname{dim} \mathbb{T}=\operatorname{dim} \mathcal{M}=\operatorname{dim} \mathcal{V}-\sum_{i=1}^{d-1} \frac{r_{i}\left(r_{i}+1\right)}{2}=\sum_{i=1}^{d} r_{i-1} n_{i} r_{i}-\sum_{i=1}^{d-1} r_{i}^{2}
$$

completing the proof.
4.2. Representations for the tangent space of $\mathbb{T}$ - main result. In approximative algorithmic treatment of high dimensional problems by means of tensor approximation, it is often the general ansatz to fix a certain tensor rank and thus a corresponding manifold $\mathcal{M}$, i.e. $\mathbb{T}_{r}$ in our case, and then to compute a - in some sense - best approximation of the solution of the problem on the given manifold $\mathcal{M}$. In many cases, knowledge of a (non-redundant) representation the tangent space $\mathcal{T}_{U} \mathcal{M}$ of this manifold is needed for the design of according algorithms, see e.g. [20, 33, 41] and also Section 6 for examples. In the remainder of this section, we shall prove the below Theorem 4.2, which gives a unique representation of the tangent space $\mathcal{T}_{U} \mathbb{T}$ taken at $U$. We will proceed as in [20,33], introducing gauge conditions to obtain uniqueness of the representation. Although these conditions are similar to the ones used for matrix case treated in [26] and for the Tucker format [27], the proof of existence and uniqueness in the present situation will be a little more subtle due to the more complicated structure of the TT tensors.

Theorem 4.2. Let $U \in \mathbb{T}$, $\delta U \in \mathcal{T}_{U} \mathbb{T}$, and let $\left(\mathbf{G}_{i}\right)_{i=1}^{d-1}$ a gauge sequence, i.e. a sequence of symmetric positive definite matrices $\mathbf{G}_{i} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)}, i=1, \ldots, d-1$.
There are unique component functions $\mathbf{W}_{i}(\cdot) \in C_{i}, i \in\{1, \ldots, d\}$, such that the tensors $\delta U_{i}$, given pointwise by

$$
\begin{equation*}
\delta U_{i}(\underline{x}):=\mathbf{U}_{1}\left(x_{1}\right) \ldots \mathbf{U}_{i-1}\left(x_{i-1}\right) \mathbf{W}_{i}\left(x_{i}\right) \mathbf{U}_{i+1}\left(x_{i+1}\right) \ldots \mathbf{U}_{d}\left(x_{d}\right), \tag{4.4}
\end{equation*}
$$

fulfil both

$$
\begin{equation*}
\delta U=\delta U_{1}+\ldots+\delta U_{d} \tag{4.5}
\end{equation*}
$$

and the gauge conditions

$$
\begin{equation*}
\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}_{i}}=\mathbf{0} \in \mathbb{R}^{r_{i} \times r_{i}} \tag{4.6}
\end{equation*}
$$

for all $i=1, \ldots, d-1$, i.e. the column vectors of the left unfoldings of $\mathbf{U}_{i}$ and $\mathbf{W}_{i}$ are orthogonal in the inner products induced by the gauging matrices $\mathbf{G}_{i}$.
These unique component functions $\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right)$ will be called the $\left(\mathbf{G}_{i}\right)$ gauged representation of $\delta U \in \mathcal{T}_{U} \mathbb{T}$.

Remark 4.3. Note that in particular, by choosing $\mathbf{G}_{i}=\mathbf{I} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)}$ for all $i=1, \ldots, d-1$, elements of the tangent space have a unique $(\mathbf{I})$-gauged representation given by component functions $\mathbf{W}_{i}: x_{i} \mapsto \mathbf{W}_{i}\left(x_{i}\right)$ for which

$$
\begin{equation*}
\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]:=\mathbf{L}\left(\mathbf{U}_{i}\right)^{T} \mathbf{L}\left(\mathbf{W}_{i}\right)=\mathbf{0} \in \mathbb{R}^{r_{i} \times r_{i}}, \tag{4.7}
\end{equation*}
$$

i.e. the column vectors of $\mathbf{L}\left(\mathbf{U}_{i}\right)$ and $\mathbf{L}\left(\mathbf{W}_{i}\right)$ are orthogonal with respect to the standard inner product on $\mathbb{R}^{r_{i-1} n_{i}}$.

To begin the proof Theorem 4.2, let $U \in \mathbb{T}$ and a gauge sequence $\left(\mathbf{G}_{i}\right)_{i=1}^{d-1}$ be given. We remind the reader that any $\delta U \in \mathcal{T}_{U} \mathbb{T}$ can be represented as the derivative of a continuously differentiable curve $\gamma$ on $\mathbb{T}$, i.e.

$$
\begin{aligned}
\mathcal{I}_{U} \mathbb{T}=\left\{\left.\gamma^{\prime}(t)\right|_{t=0} \mid \gamma \in C^{1}(]-\delta, \delta[, \mathbb{T}),\right. & \\
& \left.\gamma(t)=\mathbf{U}_{1}(\cdot, t) \cdot \ldots \cdot \mathbf{U}_{d}(\cdot, t), \quad \gamma(0)=U(\underline{x})\right\}
\end{aligned}
$$

up to isomorphisms. For technical reasons, we will at first work with the set

$$
\begin{aligned}
& \hat{\mathcal{T}}_{U} \mathbb{T}:=\left\{\left.\gamma^{\prime}(t)\right|_{t=0} \in \mathcal{T}_{U} \mathbb{T} \mid t \mapsto \mathbf{U}_{i}(\cdot, t) \text { is } C^{1}(]-\delta, \delta\left[, C_{i}\right)\right. \\
&\text { for all } i=1, \ldots, d\} \subseteq \mathcal{T}_{U} \mathbb{T}
\end{aligned}
$$

(with $C_{i}$ the spaces of component functions from (2.4)) and prove Theorem 4.2 for all $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$. At the end of this section, a dimensional argument will prove $\hat{\mathcal{T}}_{U} \mathbb{T}=\mathcal{I}_{U} \mathbb{T}$ (in contrast to the fact that there are $C^{1}$-curves $\gamma$ the components of which are not all $C^{1}$ ) - Theorem 4.2 thus holds for all $\delta U \in \mathcal{T}_{U} \mathbb{T}$ as asserted.

In Section 4.3, we prove the existence of a $\left(\mathbf{G}_{i}\right)$-gauged representation of $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$; uniqueness will be proven in Section 4.4. Finally, the equality of $\hat{\mathcal{T}}_{U} \mathbb{T}$ and $\mathcal{T}_{U} \mathbb{T}$ is subject to Section 4.5.
4.3. Proof of existence of a $\left(\mathbf{G}_{i}\right)$-gauged representation. Let $\delta U \in \hat{\mathscr{T}}_{U} \mathbb{T}$ be given. There holds for $\underline{x}=\left(x_{1}, \ldots, x_{d}\right)$,

$$
\begin{align*}
\delta U(\underline{x}) \simeq\left(\left.\gamma^{\prime}(t)\right|_{t=0}\right)(\underline{x})= & \mathbf{U}_{1}^{\prime}\left(x_{1}, 0\right) \mathbf{U}_{2}\left(x_{2}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)+ \\
& \mathbf{U}_{1}\left(x_{1}\right) \mathbf{U}_{2}^{\prime}\left(x_{2}, 0\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)+\ldots+  \tag{4.8}\\
& \mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d-1}\left(x_{d-1}\right) \mathbf{U}_{d}^{\prime}\left(x_{d}, 0\right) .
\end{align*}
$$

This yields a representation of the form (4.5) for $\delta U$; alas, the gauge condition (4.6) does not need to be satisfied. Therefore, we now utilize the following basic lemma to transform the component functions $\mathbf{U}_{1}^{\prime}(\cdot, 0), \ldots, \mathbf{U}_{d}^{\prime}(\cdot, 0)$ to a $\left(\mathbf{G}_{i}\right)$-gauged representation of $\delta U$.

Lemma 4.4. For $i \in\{1, \ldots, d\}$, let $\mathbf{M}, \mathbf{U}: \mathcal{I}_{i} \rightarrow \mathbb{R}^{r_{i-1} \times r_{i}}$ component functions, and let $\mathbf{G} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)}$ a symmetric positive definite matrix. Then there exists a unique component function $\mathbf{W} \in C_{i}, \mathbf{W}: \mathcal{I}_{i} \rightarrow \mathbb{R}^{r_{i-1} \times r_{i}}$ and a matrix $\boldsymbol{\Lambda} \in \mathbb{R}^{r_{i} \times r_{i}}$ such that

$$
\begin{equation*}
\mathbf{M}\left(x_{i}\right)=\mathbf{U}\left(x_{i}\right) \boldsymbol{\Lambda}+\mathbf{W}\left(x_{i}\right) \tag{4.9}
\end{equation*}
$$

and

$$
\begin{equation*}
[\mathbf{U}, \mathbf{W}]_{\mathbf{G}}=\mathbf{0} \in \mathbb{R}^{r_{i} \times r_{i}} \tag{4.10}
\end{equation*}
$$

i.e. the column vectors of the left unfoldings of $\mathbf{U}: x_{i} \mapsto \mathbf{U}\left(x_{i}\right)$ and $\mathbf{W}: x_{i} \mapsto \mathbf{W}\left(x_{i}\right)$ are mutually orthogonal in the inner product induced by $\mathbf{G}$. If $\mathbf{U}$ has full left rank, $\boldsymbol{\Lambda}$ is also unique.

Proof. Let $\mathbf{m}_{1}, \ldots, \mathbf{m}_{r} \in \mathbb{R}^{m}$ denote the columns of the left unfolding $\mathbf{L}(\mathbf{M})$ and $\mathbf{l}_{1}, \ldots, \mathbf{l}_{r} \in$ $\mathbb{R}^{m}$ denote the columns of $\mathbf{L}(\mathbf{U})$. For each $i \in\{1, \ldots, r\}$, we express $\mathbf{m}_{i}$ as

$$
\mathbf{m}_{i}=\sum_{j=1}^{r} \lambda_{i, j} \mathbf{l}_{j}+\mathbf{w}_{i}
$$

with suitably chosen coefficients $\lambda_{i, j} \in \mathbb{R}$ and unique $\mathbf{w}_{i} \in \mathbb{R}^{m}$ from the G-orthogonal complement of $\operatorname{span}\left\{\mathbf{l}_{1}, \ldots, \mathbf{l}_{r}\right\}$. Letting $\boldsymbol{\Lambda}=\left(\lambda_{j, i}\right)_{i, j=1}^{r}$ and $\mathbf{L}(\mathbf{W})=\left[\mathbf{w}_{1}, \ldots, \mathbf{w}_{r}\right]$ yields

$$
\mathbf{L}(\mathbf{M})=\mathbf{L}(\mathbf{U}) \boldsymbol{\Lambda}+\mathbf{L}(\mathbf{W})
$$

and thus, by applying the inverse of the left unfolding mapping $\mathbf{L}(\cdot)$, the representation (4.9). Finally, we note that if $\mathbf{U}$ has full left rank, the coefficients $\lambda_{i, j}$ also are unique.

We can now continue the proof of Theorem 4.2. We apply Lemma 4.4 to $\mathbf{G}=\mathbf{G}_{1}$, $x_{i} \mapsto \mathbf{M}\left(x_{i}\right)=U_{1}^{\prime}\left(x_{1}, 0\right), x_{i} \mapsto \mathbf{U}\left(x_{1}\right)=\mathbf{U}_{1}\left(x_{1}\right)$, and obtain that for suitable $\boldsymbol{\Lambda}_{1} \in \mathbb{R}^{r_{1} \times r_{1}}$ and a component function $\mathbf{W}_{1} \in \mathbb{R}^{n_{0} \times r_{1}}$ for which $\mathbf{W}_{1}$ is left-orthogonal to $\mathbf{U}_{1}$ in the $\mathbf{G}_{1}$-inner product (see (4.10)), the relation

$$
\mathbf{M}_{1}\left(x_{1}\right)=\mathbf{U}_{1}\left(x_{1}\right) \boldsymbol{\Lambda}_{1}+\mathbf{W}_{1}\left(x_{1}\right)
$$

holds; thus, for $\underline{x}=\left(x_{1}, \ldots x_{d}\right)$,

$$
\begin{aligned}
\delta U(\underline{x})= & \underbrace{\mathbf{W}_{1}\left(x_{1}\right) \mathbf{U}_{2}\left(x_{2}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)}_{=: \delta U_{1}(\underline{x})}+ \\
& \mathbf{U}_{1}\left(x_{1}\right)\left(\boldsymbol{\Lambda}_{1} \mathbf{U}_{2}\left(x_{2}\right)+\mathbf{U}_{2}^{\prime}\left(x_{2}, 0\right)\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)+\ldots+ \\
& \mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d-1}\left(x_{d-1}\right) \mathbf{U}_{d}^{\prime}\left(x_{d}, 0\right) .
\end{aligned}
$$

Now, we successively apply Lemma 4.4 to

$$
i=2, \ldots, d, \mathbf{G}=\mathbf{G}_{i}, \mathbf{M}_{i}\left(x_{i}\right)=\boldsymbol{\Lambda}_{i-1} \mathbf{U}_{i}\left(x_{i}\right)+\mathbf{U}_{i}^{\prime}\left(x_{i}, 0\right), \mathbf{U}\left(x_{i}\right)=\mathbf{U}_{i}\left(x_{i}\right)
$$

We obtain

$$
\begin{aligned}
\delta U(\underline{x})= & \underbrace{\mathbf{W}_{1}\left(x_{1}\right) \mathbf{U}_{2}\left(x_{2}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)}_{=: \delta U_{1}(\underline{x})}+\underbrace{\mathbf{U}_{1}\left(x_{1}\right) \mathbf{W}_{2}\left(x_{2}\right) \mathbf{U}_{3}\left(x_{3}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)}_{=: \delta U_{2}(\underline{x})} \\
& +\ldots+\underbrace{\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{d-1}\left(x_{d-1}\right)\left(\boldsymbol{\Lambda}_{d-1} \mathbf{U}_{d}\left(x_{d}\right)+\mathbf{U}_{d}^{\prime}\left(x_{d}, 0\right)\right)}_{=: \delta U_{d}(\underline{x})}
\end{aligned}
$$

for suitable $\mathbf{W}_{2}, \ldots, \mathbf{W}_{d-1}$ and $\boldsymbol{\Lambda}_{d-1}$, where (4.6) is fulfilled for all $i=1, \ldots, d-1$. Letting $\mathbf{W}_{d}\left(x_{d}\right)=\boldsymbol{\Lambda}_{d-1} \mathbf{U}_{d}\left(x_{d}\right)+\mathbf{U}_{d}^{\prime}\left(x_{d}, 0\right)$ completes the proof for
the existence of a $\left(\mathbf{G}_{i}\right)$-gauged representation for any $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$ and any gauge sequence $\left(\mathbf{G}_{i}\right)_{i=1}^{d-1}$.
4.4. Proof of uniqueness of a $\left(\mathbf{G}_{i}\right)$-gauged representation. To prove uniqueness of a $\left(\mathbf{G}_{i}\right)$-gauged representation for $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$, we will use the following lemma, which shows that it suffices to show uniqueness of representation with respect to one gauging sequence.

Lemma 4.5. Let $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$, $\left(\mathbf{G}_{i}\right)_{i=1}^{d-1},\left(\mathbf{H}_{i}\right)_{i=1}^{d-1} \quad$ be gauge sequences, and $\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right)$ and $\left(\mathbf{V}_{1}, \ldots, \mathbf{V}_{d}\right)$ be $\left(\mathbf{G}_{i}\right)-$ and $\left(\mathbf{H}_{i}\right)$-gauged representations of $\delta U$, respectively. Then, if $\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right)$ is a unique $\left(\mathbf{G}_{i}\right)$-gauged representation, $\left(\mathbf{V}_{1}, \ldots, \mathbf{V}_{d}\right)$ also is a unique $\left(\mathbf{H}_{i}\right)$-gauged representation.

Proof. Suppose that there exist two distinct $\left(\mathbf{H}_{i}\right)$-gauged representations

$$
\left(\mathbf{V}_{1}, \ldots, \mathbf{V}_{d}\right), \quad\left(\tilde{\mathbf{V}}_{1}, \ldots, \tilde{\mathbf{V}}_{d}\right)
$$

for $\delta U$. Analogously to the proceeding in the above existence proof, we use Lemma 4.4 to obtain two different $\left(\mathbf{G}_{i}\right)$-gauged representation for $\delta U$ : We again write $\delta U$ recursively as

$$
\begin{aligned}
\delta U(\underline{x})= & \sum_{j=1}^{i-1} \delta U_{j}(\underline{x})+\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot\left(\boldsymbol{\Lambda}_{i-1} \mathbf{U}_{i}\left(x_{i}\right)+\mathbf{V}_{i}\left(x_{i}\right)\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right) \\
& +\sum_{j=i+1}^{d} \mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{V}_{j}\left(x_{i}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)
\end{aligned}
$$

for $i=1, \ldots, d$, where the summands $\delta U_{j}$ are gauged with respect to the matrices $\mathbf{G}_{i}$, and as a corresponding expression for the second gauge sequence, with suitable $\left(\mathbf{G}_{i}\right)$-gauged $\delta \tilde{U}_{j}, j<i$ and $\tilde{\Lambda}_{i-1}$, and with $\tilde{\mathbf{V}}_{j}$ in place of $\mathbf{V}_{j}$ for $j \geq i$. For $i \in\{1, \ldots, d\}$ chosen minimal such that $\mathbf{V}_{i} \neq \tilde{\mathbf{V}}_{i}$, we have $\delta U_{j}=\delta \tilde{U}_{j}$ for $j<i$ and also $\boldsymbol{\Lambda}_{i-1}=\tilde{\boldsymbol{\Lambda}}_{i-1}$ due to the uniqueness of the expressions yielded by application of Lemma 4.4 (Note that $\mathbf{U}_{i}$ have full left rank by definition of $\mathbb{T}_{\underline{r}}$ ). Thus there holds

$$
\mathbf{M}_{i}\left(x_{i}\right):=\boldsymbol{\Lambda}_{i-1} \mathbf{U}_{i}\left(x_{i}\right)+\mathbf{V}_{i}\left(x_{i}\right) \neq \boldsymbol{\Lambda}_{i-1} \mathbf{U}_{i}\left(x_{i}\right)+\tilde{\mathbf{V}}_{i}\left(x_{i}\right)=: \tilde{\mathbf{M}}_{i}\left(x_{i}\right)
$$

Applying Lemma 4.4 to $\mathbf{M}_{i}, \tilde{\mathbf{M}}_{i}$ and the gauge matrix $\mathbf{G}_{i}$ gives left-orthogonal decompositions in the $\mathbf{G}_{i}$-product

$$
\mathbf{M}_{i}=\mathbf{U}_{i} \boldsymbol{\Lambda}_{i}+\mathbf{W}_{i} \neq \mathbf{U}_{i} \tilde{\boldsymbol{\Lambda}}_{i}+\tilde{\mathbf{W}}_{i}=\tilde{\mathbf{M}}_{i}
$$

for which $\boldsymbol{\Lambda}_{i} \neq \tilde{\mathbf{\Lambda}}_{i}$ or $\mathbf{W}_{i} \neq \tilde{\mathbf{W}}_{i}$ due to left-orthogonality of the summands with respect to the $\mathbf{G}_{i}$-product. An easy inductive argument now shows that if we proceed as in the above existence proof to obtain $\left(\mathbf{G}_{i}\right)$-gauged representations, this implies $\delta U_{j} \neq \delta \tilde{U}_{j}$ for some $j \geq i$, finishing the proof.

To complete the proof of Theorem 4.2, we note that the matrices

$$
\begin{equation*}
\mathbf{G}_{i}:=\llbracket U, U \rrbracket \rrbracket^{\leq i-1} \otimes \mathbf{I}_{n_{i} \times n_{i}} \in \mathbb{R}^{\left(r_{i-1} n_{i}\right) \times\left(r_{i-1} n_{i}\right)} \tag{4.11}
\end{equation*}
$$

defined in (3.11) form a gauge sequence by Lemma 3.4; we will now show that for this particular gauge sequence, the $\left(\mathbf{G}_{i}\right)$-gauged representation of $\delta U$ is unique. As a final preparation for the proof thereof, we give a decomposition for $\langle V, W\rangle$ in the following remark.

Remark 4.6. Let $V, W \in \mathbb{T}$ be tensors, and let $\langle\cdot, \cdot \cdot\rangle$ denote the usual Euclidean inner product on $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$. By splitting up $\llbracket V, W \rrbracket^{\leq d}$ into an $i$-left and $i+1$-th right part, it is not hard to see (e.g. by writing out sums or by usage of the diagrams for $\llbracket V, W \rrbracket \leq i$, $\llbracket V, W \rrbracket^{\geq i+1}$ ) that

$$
\begin{aligned}
\langle V, W\rangle & =\llbracket V, W \rrbracket^{\leq d}=\langle\underbrace{\llbracket V, W \rrbracket}_{\in \mathbb{R}^{r_{i} \times r_{i}}}, \underbrace{\llbracket V, W \rrbracket^{\geq i+1}}_{\in \mathbb{R}^{r_{i} \times r_{i}}}\rangle \\
& =\left\langle\left(\mathbf{L}\left(\mathbf{W}_{i}\right)^{T}\left(\llbracket V, W \rrbracket^{(\leq i-1)} \otimes \mathbf{I}_{n_{i} \times n_{i}}\right) \mathbf{L}\left(\mathbf{V}_{i}\right), \llbracket V, W \rrbracket^{\geq i+1}\right\rangle,\right.
\end{aligned}
$$

in which the last line follows from (3.10). In particular, if for some $j \in\{1, \ldots, d\}, V$ and $W$ coincide in the first $j-1$ components, i.e.

$$
\begin{aligned}
V(\underline{x}) & =\mathbf{U}_{1}\left(x_{1}\right) \ldots \mathbf{U}_{j-1}\left(x_{j-1}\right) \mathbf{V}_{j}\left(x_{j}\right) \ldots \mathbf{V}_{d}\left(x_{d}\right) \\
W(\underline{x}) & =\mathbf{U}_{1}\left(x_{1}\right) \ldots \mathbf{U}_{j-1}\left(x_{j-1}\right) \mathbf{W}_{j}\left(x_{j}\right) \ldots \mathbf{W}_{d}\left(x_{d}\right)
\end{aligned}
$$

for some component functions $\mathbf{U}_{i}\left(x_{i}\right)$, then for all $i \leq j$

$$
\begin{align*}
\langle V, W\rangle & :=\left\langle\left(\mathbf{L}\left(\mathbf{W}_{i}\right)^{T} \mathbf{G}_{i} \mathbf{L}\left(\mathbf{V}_{i}\right), \llbracket V, W \rrbracket^{\geq i+1}\right\rangle\right.  \tag{4.12}\\
& =\left\langle\left[\mathbf{V}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}_{i}}, \llbracket V, W \rrbracket^{\geq i+1}\right\rangle
\end{align*}
$$

with $\mathbf{G}_{i}$ defined as by (4.11).

We are now in the position to prove uniqueness of the $\left(\mathbf{G}_{i}\right)$-gauged representation

$$
\begin{align*}
& \delta U=\sum_{i=1}^{d} \delta U_{i}  \tag{4.13}\\
& \delta U_{i}(\underline{x})=\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{i-1}\left(x_{i-1}\right) \mathbf{W}_{i}\left(x_{i}\right) \mathbf{U}_{i+1}\left(x_{i+1}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right)
\end{align*}
$$

for $\delta U \in \hat{\mathcal{T}}_{U} \mathbb{T}$, where the component functions $\mathbf{W}_{i}$ fulfil the gauge condition (4.6) with the gauge sequence $\left(\mathbf{G}_{i}\right)$ defined via (4.11) by the tensor $U$. To do so, we have to show that for $i=1 \ldots, d$, the component functions $\mathbf{W}_{i}$ are uniquely determined by $\delta U$. We start by noting that $\mathbf{W}_{i}$ is uniquely determined iff $\mathbf{L}\left(\mathbf{W}_{i}\right)$ is unique, which in turn by Lemma 3.4 is the case iff the matrix

$$
\mathbf{G}_{i} \mathbf{L}\left(\mathbf{W}_{i}\right) \mathbf{P}_{i+1} \in \mathbb{R}^{\left(r_{i-1} \cdot n_{i}\right) \times r_{i}}
$$

is uniquely determined (where we let $\mathbf{G}_{1}=\mathbf{I}_{n_{1} \times n_{1}}$ and $\mathbf{P}_{d+1}=(1) \in \mathbb{R}^{1 \times 1}$ for convenience). Cast into a weak formulation, this is the case if and only if for any component function $\mathbf{V}_{i}: \mathbb{R}^{n_{i}} \rightarrow \mathbb{R}^{\left(r_{i-1} \times r_{i}\right)}$, the Euclidean inner product

$$
\begin{equation*}
\left\langle\mathbf{G}_{i} \mathbf{L}\left(\mathbf{W}_{i}\right) \mathbf{P}_{i+1}, \mathbf{L}\left(\mathbf{V}_{i}\right)\right\rangle=\left\langle\mathbf{L}\left(\mathbf{V}_{i}\right)^{T} \mathbf{G}_{i} \mathbf{L}\left(\mathbf{W}_{i}\right), \mathbf{P}_{i+1}\right\rangle \tag{4.14}
\end{equation*}
$$

(taken on $\mathbb{R}^{r_{i-1} n_{i} r_{i-1}}$ ) is uniquely determined by $\delta U$. If we define for any component function $\mathbf{V}_{i}$ a corresponding tensor

$$
\begin{equation*}
V_{i}(\underline{x}):=\mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{i-1}\left(x_{i-1}\right) \mathbf{V}_{i}\left(x_{i}\right) \mathbf{U}_{i+1}\left(x_{i+1}\right) \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right), \tag{4.15}
\end{equation*}
$$

we can use (4.12), (4.13) and (4.15) to rewrite (4.14) as

$$
\begin{equation*}
\left\langle\left(\mathbf{L}\left(\mathbf{V}_{i}\right)\right)^{T} \mathbf{G}_{i} \mathbf{L}\left(\mathbf{W}_{i}\right), \mathbf{P}_{i+1}\right\rangle=\left\langle\delta U_{i}, V_{i}\right\rangle, \quad \text { for all } \mathbf{V}_{i} \in C_{i} \tag{4.16}
\end{equation*}
$$

and we now use the gauge condition to show that for fixed test component function $\mathbf{V}_{i},\left\langle\delta U_{i}, V_{i}\right\rangle$ is indeed uniquely determined by $\delta U$. To this end, we observe that for all $1 \leq j<i \leq d$,

$$
\left\langle\delta U_{j}, V_{i}\right\rangle=\left\langle\left(\mathbf{L}\left(\mathbf{W}_{j}\right)\right)^{T} \mathbf{G}_{j} \mathbf{L}\left(\mathbf{U}_{j}\right), \llbracket \delta U_{j}, V_{i} \rrbracket^{\leq j+1}\right\rangle=0 \quad \text { for all } \mathbf{V}_{i} \in C_{i}
$$

by (4.12) and the gauge condition (4.6), and that therefore

$$
\begin{equation*}
\left\langle\delta U, V_{i}\right\rangle=\sum_{j=i}^{d}\left\langle\delta U_{j}, V_{i}\right\rangle, \quad \text { for all } i=1, \ldots, d \tag{4.17}
\end{equation*}
$$

Starting with $i=d$, we obtain the uniquely solvable linear equation

$$
\left\langle\left(\mathbf{L}\left(\mathbf{V}_{d}\right)\right)^{T} \mathbf{G}_{d} \mathbf{L}\left(\mathbf{W}_{d}\right), \mathbf{P}_{d+1}\right\rangle=\left\langle\delta U, V_{d}\right\rangle
$$

for $\mathbf{L}\left(\mathbf{W}_{d}\right)$, with the right hand side fixed by $\delta U$. We now proceed recursively: Once $\mathbf{L}\left(\mathbf{W}_{i}\right)$ and thus $\mathbf{W}_{i}, i=d, d-1, \ldots$, is computed, the values $\left\langle\delta U_{i}, V_{i}\right\rangle$ are computable. $\mathbf{W}_{i-1}$ is then fixed by (4.16) with

$$
\begin{equation*}
\left\langle\delta U_{i}, V_{i}\right\rangle=\left\langle\delta U, V_{i}\right\rangle-\sum_{j=i+1}^{d}\left\langle\delta U_{j}, V_{i}\right\rangle, \quad \text { for all } i=d, \ldots, 1, \tag{4.18}
\end{equation*}
$$

uniquely determining the right hand side, so that $\mathbf{L}\left(\mathbf{W}_{i-1}\right)$ and thus $\mathbf{W}_{i-1}$ are unique as solution of (4.16).

Remark 4.7. We note that the preceeding proof mainly relies on the fact that the full-rank-condition imposed on the TT decomposition of $U$ implies that the matrices $\mathbf{G}_{i}, \mathbf{P}_{i+1}$ are symmetric and positive definite by Lemma 3.4, thus allowing for a unique solution of the weak equations yielded by (4.17). Those equations can be restated as

$$
\begin{equation*}
\left\langle\left(\mathbf{G}_{i} \otimes \mathbf{P}_{i+1}\right) \operatorname{vec}\left(\mathbf{W}_{i}\right), \operatorname{vec}\left(\mathbf{V}_{i}\right)\right\rangle=\left\langle\delta U_{i}, V_{i}\right\rangle \tag{4.19}
\end{equation*}
$$

in which $\operatorname{vec}\left(\mathbf{U}_{i}\right)$ denotes the vectorisation of a component function $\mathbf{U}_{i}$. The matrices $\mathbf{G}_{i}, \mathbf{P}_{i+1}$, often termed density matrices in the context of quantum physics and DMRG calculations, thus play a role similar to that of the analogous density matrices in [27].
In practical TT computations, the treatment of problems as computation of best approximations or solution of linear equations often boils down to solution of equations similar to (4.19); in particular, when computing the $i$-th component of a best approximation, one can choose the component functions $\mathbf{U}_{j}$ left-orthogonal for $j<i$ and right-orthogonal for $j>i$, so that the density matrices are given by the identity. See the forthcoming publication [21] for further details.
4.5. A parametrization of the tangent space $\mathcal{T}_{U} \mathbb{T}$. Finally, we now show $\hat{\mathcal{T}}_{U} \mathbb{T}=\mathcal{T}_{U} \mathbb{T}$, by which Theorem 4.2 is then proven. To this end, observe at first that $\operatorname{dim} \mathcal{T}_{U} \mathbb{T}=\operatorname{dim} \mathbb{T}$ is given by (4.2). We show that $\hat{\mathcal{T}}_{U} \mathbb{T} \subseteq \operatorname{dim} \mathcal{T}_{U} \mathbb{T}$ possesses the same dimension, thus proving $\hat{\mathcal{T}}_{U} \mathbb{T}=\mathcal{T}_{U} \mathbb{T}$. The more general statement of the below Lemma 4.8 will also be useful in the next section. At first, we define within the spaces $C_{i}$ of component functions the (linear) left-orthogonal spaces of $\mathbf{U}_{i}$,

$$
U_{i}^{\ell}:=\left\{\mathbf{W}_{i} \in C_{i},\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}_{i}}=\mathbf{0}\right\}
$$

for $1 \leq i \leq d-1$, and

$$
\begin{equation*}
X:=U_{1}^{\ell} \times \ldots \times U_{d-1}^{\ell} \times C_{d} \tag{4.20}
\end{equation*}
$$

Obviously, due to the $r_{i}$ orthogonality constraints imposed on each of the column vectors of $\mathbf{L}\left(\mathbf{W}_{i}\right)$ for $i \in\{1, \ldots, d-1\}$

$$
\begin{gathered}
\operatorname{dim} U_{i}^{\ell}=r_{i-1} n_{i} r_{i}-r_{i}^{2} ; \quad \text { and } \quad \operatorname{dim} C_{d}=r_{d-1} n_{d} \\
\operatorname{dim} X=\sum_{i=1}^{d} r_{i-1} n_{i} r_{i}-\sum_{i=1}^{d-1} r_{i}^{2}
\end{gathered}
$$

The following lemma is now an immediate corollary of the existence and uniqueness results proven in Section 4.3 and 4.4.

Lemma 4.8. The mapping

$$
\begin{equation*}
\tau: X \rightarrow \hat{\mathcal{T}}_{U} \mathbb{T},\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right) \mapsto \delta U \tag{4.21}
\end{equation*}
$$

where

$$
\delta U(\underline{x})=\sum_{i=1}^{d} \mathbf{U}_{1}\left(x_{1}\right) \cdot \ldots \cdot \mathbf{U}_{i-1}\left(x_{i-1}\right) \mathbf{W}_{i}\left(x_{i}\right) \mathbf{U}_{i+1}\left(x_{i+1}\right) \cdot \ldots \cdot \mathbf{U}_{d}\left(x_{d}\right),
$$

is a linear bijection between $X$ and the tangent space $\mathcal{T}_{U} \mathbb{T}$, taken at $U$. In particular,

$$
\begin{equation*}
\operatorname{dim} \hat{\mathcal{T}}_{U} \mathbb{T}=\operatorname{dim} \mathcal{T}_{U} \mathbb{T}, \quad \hat{\mathcal{T}}_{U} \mathbb{T}=\mathcal{I}_{U} \mathbb{T} \tag{4.22}
\end{equation*}
$$

## 5. A Local parametrization for the manifold $\mathbb{T}$

In this section, we use the just proven representation

$$
\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right) \in X, \quad \text { i.e. } \quad\left[\mathbf{U}_{i}, \mathbf{W}_{i}\right]_{\mathbf{G}_{i}}=\mathbf{0}
$$

for $\mathcal{I}_{U} \mathbb{T}$ and the statement given in Lemma 4.8 to set up a local parametrization of $\mathbb{T}$ and to define local charts for $\mathbb{T}$. The results are collected in Theorem 5.2. As before, we fix $U \in \mathbb{T}$ and a gauging sequence $\left(\mathbf{G}_{i}\right)$.

Lemma 5.1. Let $X$ be defined as in (4.20), and let

$$
\Psi: X \rightarrow \mathbb{R}^{n_{1} \times \ldots \times n_{d}},\left(\mathbf{W}_{1}, \ldots, \mathbf{W}_{d}\right) \mapsto \quad\left(\mathbf{U}_{1}+\mathbf{W}_{1}\right) \cdot \ldots \cdot\left(\mathbf{U}_{d}+\mathbf{W}_{d}\right)
$$

where the matrix product representation is understood pointwise as above. There is an open neighbourhood $N_{\delta}=N_{\delta}(0)$ of $0 \in X$ such that $\Psi\left(N_{\delta}\right)$ is an open subset of $\mathbb{T}$, and such that the restriction

$$
\begin{equation*}
\left.\Psi\right|_{N_{\delta}}: N_{\delta} \mapsto \Psi\left(N_{\delta}\right) \tag{5.2}
\end{equation*}
$$

is a diffeomorphism.

Proof. We utilize the inverse mapping theorem for manifolds, cf. e.g. [32], Theorem 2.25. We note at first that with the same arguments as in the proof of Lemma 4.1, restriction of $\Psi$ to a suitable open neighbourhood $\tilde{N}$ of 0 gives a mapping $\Psi: \tilde{N} \rightarrow \Psi(\tilde{N}) \subseteq \mathbb{T}$. A straightforward computation shows that the tangent map $T_{U} \Psi$ belonging to $\Psi$ (also see e.g. [32]) is given by the bijection (4.21). Thus the conditions of the inverse mapping theorem for manifolds are fulfilled, yielding the asserted statement.

Because of Lemma 4.8, any set $\mathcal{C}=\left(\mathcal{C}_{1}, \ldots, \mathcal{C}_{d}\right)$ of coordinate mappings $\mathcal{C}_{i}: U_{i}^{\ell} \rightarrow$ $\mathbb{R}^{r_{i-1} n_{i} r_{i}-r_{i}^{2}}$ for $i=1, \ldots, d-1, \mathcal{C}_{d}: C_{d} \rightarrow \mathbb{R}^{r_{d-1} n_{d}}$, defines an isomorphism between $X$ and $\mathbb{R}^{D}$,

$$
D:=\sum_{i=1}^{d} r_{i-1} n_{i} r_{i}-\sum_{i=1}^{d-1} r_{i}^{2} .
$$

We can therefore combine (5.1) with the coordinate mappings to obtain a local parametrization of $\mathbb{T}$ by letting $\mathcal{C}=\left(\mathcal{C}_{1}, \ldots, \mathcal{C}_{d}\right), \psi:=\mathcal{C}^{-1} \circ \Psi: \mathbb{R}^{D} \rightarrow \mathbb{T}$. The properties of this parametrization and some more implications are collected in the next theorem, finishing this section.

Theorem 5.2. For all $U \in \mathbb{T}$, there exists an open neighbourhood $N_{U} \subset \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ of $U$, an open neighbourhood $N_{\delta}(0)$ of $0 \in \mathbb{R}^{D}$ and differentiable functions

$$
\psi=\psi_{U}: N_{\delta}(0) \rightarrow \mathbb{R}^{n_{1} \times \ldots, \times n_{d}}, \quad g=g_{U}: N_{U} \rightarrow \mathbb{R}^{c}, c:=\sum_{i=1}^{d-1} r_{i}^{2}
$$

such that

$$
\begin{equation*}
N_{U} \cap \mathbb{T}=\psi\left(N_{\delta}(0)\right)=\left\{U \in \mathbb{R}^{n_{1} \times \ldots, \times n_{d}}: g(U)=0\right\} \tag{5.3}
\end{equation*}
$$

and the above parametrisation $\psi$ 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 $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$.

Proof. The local parametrization $\psi$ was already constructed above. The proof of Lemma 5.1 shows that the tangent mapping of $\psi$ is an injection, making $\psi$ an immersion. Lemma 5.1 also states that $\psi$ is a homeomorphism onto its image. This also implies the existence of a local constraint function $g$ characterizing $\mathbb{T}$ on a neighbourhood of $U$, see e.g. [20], IV.5.1. The last statement follows from the fact that $\psi$ is an embedding, cf. e.g. [32], Theorem 3.5.

## 6. Examples of problems posed on the manifold of TT tensors

To illustrate the range of applications, we now review a well-known ansatz [20, 26, 33] for how partial differential equations and optimisation problems posed in high-dimensional spaces $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ may be solved approximately on a given approximation manifold, in our case on the manifold $\mathbb{T}$ of TT tensors.

Let a differential equation

$$
\begin{equation*}
\frac{d u}{d t}=f(u) \tag{6.1}
\end{equation*}
$$

for a high dimensional function $u: t \mapsto u(t) \in \mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ be given, e.g. stemming from the Galerkin discretization time-dependent PDE formulated on a high-dimensional function space. Our goal is the approximation of the solution $u$ by a (usually much more sparsely representable) TT tensor-valued function $U(t) \in \mathbb{T}=\mathbb{T}(\underline{r})$ of fixed rank $\underline{r}$ chosen in advance. To this end, we replace the equation (6.1) by a related differential equation posed on the approximation manifold $\mathbb{T}$, i.e. for all starting values $U(0)=U_{0} \in \mathbb{T}$, the solution fulfils $U(t) \in \mathbb{T}$. This is achieved as follows: If a manifold $\mathbb{T}$ possesses a local embedding $\psi=\psi_{U}$ for each $U \in \mathbb{T}$, as the TT manifold does by Theorem 5.2, a differential equation $\dot{U}=F(U)$ is a differential equation on $\mathbb{T}$ if and only if

$$
F(U) \in \mathcal{T}_{U} \mathbb{T}
$$

holds for all $U \in \mathbb{T}$, see e.g. [20], Theorem 5.2; in particular, we have $U(t) \in \mathbb{T}$ for all $t>0$. Therefore, (6.1) can be solved approximately by projecting $f(U)$ on the tangent space $\mathcal{T}_{U} \mathbb{T}$ for each $U \in \mathbb{T}$, i.e. by defining

$$
F(U):=P_{T_{U}} f(U) \in \mathcal{T}_{U} \mathbb{T}
$$

where $P_{\mathcal{T}_{U}}$ projects on the tangent space $\mathcal{T}_{U} \mathbb{T}$, and by then solving the projected differential equation

$$
\begin{equation*}
\frac{d U}{d t}=F(U) \tag{6.2}
\end{equation*}
$$

that, by the above reasoning, is a differential equation posed on the manifold $\mathbb{T}$. Note that the solution $U(t)$ is a curve in $\mathbb{T}$, so by definition $d U / d t$ is contained in the tangent space $\mathcal{T}_{U} \mathbb{T}$. Thus $P_{\tau_{U}} d U / d t=d U / d t$, which implies that

$$
\begin{equation*}
\frac{d U}{d t}-F(U)=0 \quad \Longleftrightarrow \quad\left\langle\frac{d U}{d t}-f(U), \delta U\right\rangle=0 \quad \text { for all } \quad \delta U \in \mathcal{T}_{U} \mathbb{T} \tag{6.3}
\end{equation*}
$$

i.e. (6.2) can therefore be interpreted as the Galerkin projection of the original problem onto the state dependent test space $\mathcal{I}_{U} \mathbb{T}$. In the context of time-dependent quantum
chemistry, the above proceeding is well-known as the Dirac-Frenkel time dependent variational principle, see [33]. The projected problem can now be solved by applying standard methods [30] to the equivalent differential equation

$$
\begin{equation*}
\frac{d z}{d t}=\tau^{-1}(F(\psi(z))) \tag{6.4}
\end{equation*}
$$

with $\tau$ from (4.21) and $\psi$ being a local parametrization. On the whole, problem (6.1) on $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ is thus replaced by a differential equation in the (linear, much lower-dimensional) coordinate space $\mathbb{R}^{D}$, also cf. [20] for details.

The above problem of solving the partial differential equation (6.1) includes the noteworthy special case of the standard minimisation problem

$$
\begin{equation*}
\mathcal{J}(u) \rightarrow \min \quad \text { for differentiable } \mathcal{J}: \mathbb{R}^{n_{1} \times \ldots \times n_{d}} \rightarrow \mathbb{R} \tag{6.5}
\end{equation*}
$$

which by the choices

$$
\mathcal{J}(u)=\frac{\langle A u, u\rangle}{\langle u, u\rangle}, \quad \mathcal{J}(u)=\|A u-b\|^{2}, \quad \mathcal{J}(u)=\|f(u)\|^{2}
$$

for instance includes the problem of finding the lowest eigenvalue for a symmetric positive definite $A$, solution of linear equations for such $A$, nonlinear equations and also, by letting $A=\hat{A}^{\frac{1}{2}}$ for $\hat{A}>0, b=\hat{A}^{\frac{1}{2}} \hat{b}$, the problem of finding a best approximation to given $\hat{b}$ with respect to the $\hat{A}$ inner product. Defining the gradient flow of $\mathcal{J}$ by the differential equation

$$
\begin{equation*}
\frac{d u}{d t}=-\mathcal{J}^{\prime}(u) \tag{6.6}
\end{equation*}
$$

the problem (6.5) is equivalent to computation of the long-term behaviour $\lim _{t \rightarrow \infty} u(t)$ of a solution of (6.6). The variational formulation on $\mathbb{T}$, obtained in the above way, reads

$$
\begin{equation*}
\left\langle\frac{d U}{d t}+\mathcal{J}^{\prime}(U), \delta U\right\rangle=0 \quad \text { for all } \quad \delta U \in \mathcal{T}_{U} \mathbb{T} \tag{6.7}
\end{equation*}
$$

and a solution $U(t) \in \mathbb{T}$ to (6.6) can be computed by the above mentioned methods.

## 7. Numerical examples

In this section, we present some numerical experiments for the TT format. We compare two different approaches to obtain a TT tensor representation from a given full tensor: One is the full_to_tt method from the TT-Toolbox, introduced in [34]. The method creates a TT tensor by computation of successive SVDs, afterwards truncated at a chosen bound relative to the Frobenius norm of the full tensor. The second algorithm is a
modified alternating least square algorithm inspired by the DMRG algorithm used in quantum physics, where in each inner iteration, two component functions are optimized and then decomposed by truncated SVDs to update one of the component functions. The algorithm, starting with a random TT approximation of rank one and referred to as MALS in the following, will be discussed at more length in a forthcoming paper [21]. The bound for the SVD truncations was set to $10^{-12}$ in full_to_tt and to $10^{-9}$ for MALS. All algorithms were implemented in Matlab using only the build-in functions and the TT-Toolbox [37], using an AMD processor with four $2,6 \mathrm{GHz}$ cores and a total 16 GB RAM. In the following we describe two experiments. They confirm that the full_to_tt method works stably due to the use of SVDs; also, in contrast to ALS for the canonical format, the MALS variation for TT works very well in many cases: It seems to be as stable as the direct SVD full_to_tt method, while often being much faster than full_to_tt.


Figure 6. TT approximations of random tensors of different ranks $r$.
7.1. Restoring a tensor with specific TT rank. In the first experiment, we converted a TT tensor of given rank $\underline{r}$ to a full tensor in $\mathbb{R}^{n_{1} \times \ldots \times n_{d}}$ and investigated if the full tensor is restored by a full_to_tt/MALS TT approximation of the same rank. As appoximand, we used tensors of ranks $\underline{r}$ with $r_{i}=r=1, \ldots, 25$ for $i=2, \ldots, d-2, r_{1}=r_{d-1}=\min \left\{r, n_{1}\right\}$, having order $d=10$, spatial dimensions $n_{1}=\ldots=n_{d}=5$ and Frobenius norm 100. Both methods gave back a tensor with the same rank as the initial random tensor in all cases, where MALS only needed one iteration step in all experiments. The results are displayed in

Fig. 6. Plot (a) shows the absolute error of the approximation. The precision is measured by the function tt_dist_2 from the TT toolbox, giving back the Frobenius norm of the distance between two TT tensors. While both are sufficiently close to machine precision, the MALS method is about 10 times more precise than full_to_tt. Plot (b) shows the time needed to compute the TT decomposition. Here, the advantage of the MALS variation becomes apparent: With growing rank, the SVDs used in full_to_tt have to be computed for increasingly bigger matrices, while for MALS, the growth of computational resources needed is moderate.


Figure 7. TT approximations of Friedman data sets.
7.2. Variation of the Friedman1 data set. In the second experiment, we approximated synthetic data obtained from the combination of continuous functions. We use a variation of the Friedman1 data set [17] for example used in [6]. For $d=5$ and $n_{i}=n$ with $n \in\{3, \ldots, 20\}$, we use index sets

$$
\mathcal{I}_{1}^{(n)}=\ldots=\mathcal{I}_{5}^{(n)}=\left\{\left.\frac{k}{n} \right\rvert\, k=0, \ldots, n\right\} .
$$

We approximate the tensor given by

$$
\begin{aligned}
& U^{(n)}: \mathcal{I}_{1}^{(n)} \times \ldots \times \mathcal{I}_{5}^{(n)} \rightarrow \mathbb{R} \\
& U(\underline{x})=10 \sin \left(\pi x_{1} x_{2}\right)+20\left(x_{3}-0.5\right)^{2}+10 x_{4}+5 x_{5}
\end{aligned}
$$

Note that the Frobenius norm of $U$ grows exponentially with $n$, see Fig. 7 (a). The algorithms full_to_tt and MALS both produce TT approximations with ranks $r_{2}=r_{3}=$ $r_{4}=2$. The results for $r_{1}$ are depicted in Fig. 7 (b). In (c), the absolute approximation errors (in the Frobenius norm) are displayed. The plot (b) shows that for some values of $n$, MALS computes an approximation for which the rank $r_{1}$ is bigger than that computed by full_to_tt, corresponding a better approximation precision in (c). Figure (d) compares the computation times needed for both decompositions.

## 8. Conclusion

We have shown that the set $\mathbb{T}_{\underline{r}}$ of tensors of fixed TT rank, being the simplest special case of the hierarchical HT format [19], locally forms an embedded submanifold of $\mathbb{R}^{n^{d}}$. This is analogous to according results for the Tucker format [27], and similar methods for the approximation of high dimensional problems as differential equations and optimisation problems may now be utilized. In particular, we have parametrized the tangent spaces of $\mathbb{T}$ uniquely by introducing appropriate gauge conditions similar to those in [33]. Thus, persuing the quasi-Galerkin approach introduced in Section 6, the according projectors on the respective tangent spaces - needed for a numerical treatment in this vein - may now be computed explicitly. Although we have only recently started the development and implementation of such algorithms, our preliminary numerical examples given in this paper show that in practice, the stability of TT format is competitive with the Tucker format; in particular, the MALS algorithm, being closely related to the DMRG approach successfully applied in quantum chemistry, shows some advantages in comparison with the ALS approach. Its potential for the treatment of high-dimensional problems will be explored further in a forthcoming publication.

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