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Abstract

Various tensor formats are used for the data-sparse representation of large-scale tensors. Here we investigate how symmetric or antiymmetric tensors can be represented. The analysis leads to several open questions.

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1 Introduction

We consider tensor spaces of huge dimension exceeding the capacity of computers. Therefore the numerical treatment of such tensors requires a special representation technique which characterises the tensor by data of moderate size. These representations (or formats) should also support operations with tensors. Examples of operations are the addition, the scalar product, the componentwise product (Hadamard product), and the matrix-vector multiplication. In the latter case, the 'matrix' belongs to the tensor space of Kronecker matrices, while the 'vector' is a usual tensor.

In certain applications the subspaces of symmetric or antisymmetric tensors are of interest. For instance, fermionic states in quantum chemistry require antisymmetry, whereas bosonic systems are described by symmetric tensors. The appropriate representation of (anti)symmetric tensors is seldom discussed in the literature. Of course, all formats are able to represent these tensors since they are particular examples of general tensors. However, the special (anti)symmetric format should exclusively produce (anti)symmetric tensors. For instance, the truncation procedure must preserve the symmetry properties.

The formats in use are the *r*-term format (also called the canonical format), the subspace (or Tucker) format, and the hierarchical representation including the TT format. In the general case, the last format has turned out to be very efficient and flexible. We discuss all formats concerning application to (anti)symmetric tensors.

The r-term format is seemingly the simplest one, but has several numerical disadvantages. In §2 we discuss two different approaches to representing (anti)symmetric tensors. However, they inherit the mentioned disadvantages.

As explained in §3, the subspace (or Tucker) format is not helpful.

The main part of the paper discusses the question how the TT format can be adapted to the symmetry requirements. The analysis leads to unexpected difficulties. In contrast to the general case, the subspaces U_j involved in the TT format (see §4.3) have to satisfy conditions which are not easy to check. We can distinguish the following two different situations.

In the first case we want to construct the TT format with subspaces \mathbf{U}_j not knowing the tensor \mathbf{v} to be represented in advance. For instance we change \mathbf{U}_j to obtain a variation of \mathbf{v} , or the dimension of \mathbf{U}_j is reduced to obtain a truncation. In these examples, \mathbf{v} is obtained as a result on the chosen \mathbf{U}_j . It turns out that the choice of \mathbf{U}_j is delicate. If \mathbf{U}_j is too small, no nontrivial tensors can be represented. On the other hand, \mathbf{U}_j may contain a useless nontrivial part, i.e., \mathbf{U}_j may be larger than necessary. The algebraic characterisation of the appropriate \mathbf{U}_j is rather involved.

In the second case, we start from \mathbf{v} and know the minimal subspaces $\mathbf{U}_{j}^{\min}(\mathbf{v})$ (cf. (1.9)). Then $\mathbf{U}_{j}^{\min}(\mathbf{v}) \subset \mathbf{U}_{j}$ is a sufficient condition. However, as soon as we want to truncate the tensor \mathbf{v} , its result \mathbf{v}' must be determined from modified subspaces \mathbf{U}_{j}' so that we return to the difficulties of the first case.

In Section 8 we describe the combination of the TT format and the ANOVA technique for symmetric tensors. This leads to a favourable method as long as the ANOVA degree is moderate.

Quite another approach for antisymmetric tensors is the so-called 'second quantisation' (cf. Legeza et al. [12, §2.3]) which does not fit into the following schemes.

1.1 Tensor Notation

1.1.1 Tensors Spaces

In the general case, vector spaces V_j $(1 \le j \le d)$ are given which determine the algebraic tensor space $\mathbf{V} := \bigotimes_{j=1}^d V_j$. The common underlying field of the vector spaces V_j is either \mathbb{R} or \mathbb{C} . In the following we write \mathbb{K} for either of the fields. In the particular case of

$$V_j = V \qquad \text{for all } 1 \le j \le d \tag{1.1}$$

we write $\mathbf{V} := \otimes^d V$. Set

$$D := \{1, \dots, d\}$$
(1.2)

and consider any nonempty subset $\alpha \subset D$. We set

$$\mathbf{V}_{\alpha} := \bigotimes_{j \in \alpha} V_j \,. \tag{1.3}$$

Note that $\mathbf{V} = \mathbf{V}_D$ is isomorphic to $\mathbf{V}_{\alpha} \otimes \mathbf{V}_{D \setminus \alpha}$.

We assume that V is a pre-Hilbert space with the scalar product $\langle \cdot, \cdot \rangle$. Then **V** and each \mathbf{V}_{α} is defined as a pre-Hilbert space with the induced scalar product uniquely defined by (cf. [9, Lemma 4.124])

$$\left\langle \bigotimes_{j \in \alpha} v^{(j)}, \bigotimes_{j \in \alpha} w^{(j)} \right\rangle = \prod_{j \in \alpha} \left\langle v^{(j)}, w^{(j)} \right\rangle.$$
(1.4)

1.1.2 Functionals

Let $\varphi_{\alpha} \in \mathbf{V}'_{\alpha}$ be a linear functional. The same symbol φ_{α} is used for the linear map $\varphi_{\alpha} : \mathbf{V} \to \mathbf{V}_{D \setminus \alpha}$ defined by

$$\varphi_{\alpha}\left(\bigotimes_{j=1}^{d} v^{(j)}\right) = \varphi_{\alpha}\left(\bigotimes_{j\in\alpha} v^{(j)}\right)\bigotimes_{j\in D\setminus\alpha} v^{(j)}$$
(1.5)

(it is sufficient to define a linear map by its action on elementary tensors, cf. [9, Remark 3.55]). In the case of (1.1) and $\varphi \in V'$ we introduce the following notation. The linear mapping $\varphi^{(k)} : \otimes^d V \to \otimes^{d-1} V$ is defined by

$$\varphi^{(k)}\left(\bigotimes_{j=1}^{d} v^{(j)}\right) = \varphi\left(v^{(k)}\right)\bigotimes_{j \neq k} v^{(j)}.$$
(1.6)

1.1.3 Permutations and (Anti)symmetric Tensor Spaces

A permutation $\pi \in P_d$ is a bijection of D onto itself. For $\nu, \mu \in D$, the permutation $\pi_{\nu\mu}$ is the transposition swapping the positions ν and μ . If $\nu = \mu$, $\pi_{\nu\mu}$ is the identity id. Let $\mathbf{V} = \otimes^d V$. Then the symbol of the permutation π is also used for the linear map $\pi : \mathbf{V} \to \mathbf{V}$ defined by

$$\pi\left(\bigotimes_{j=1}^{d} v^{(j)}\right) = \bigotimes_{j=1}^{d} v^{(\pi^{-1}(j))}$$

Each permutation π is a (possibly empty) product of transpositions: $\pi = \pi_{\nu_1 \mu_1} \circ \pi_{\nu_2 \mu_2} \circ \ldots \circ \pi_{\nu_k \mu_k}$ with $\nu_i \neq \mu_i$ $(1 \leq i \leq k)$. The number k determines the parity ± 1 of the permutation: $\operatorname{sign}(\pi) = (-1)^k$.

A tensor $\mathbf{v} \in \otimes^d V$ is called *symmetric* if $\pi(\mathbf{v}) = \mathbf{v}$ for all permutations, and antisymmetric if $\pi(\mathbf{v}) = \operatorname{sign}(\pi)\mathbf{v}$. This defines the (anti)symmetric tensor space:

$$\mathbf{V}_{\text{sym}} := \left\{ \mathbf{v} \in \otimes^d V : \pi(\mathbf{v}) = \mathbf{v} \right\},\tag{1.7a}$$

$$\mathbf{V}_{\text{anti}} := \left\{ \mathbf{v} \in \otimes^d V : \pi(\mathbf{v}) = \operatorname{sign}(\pi) \mathbf{v} \right\}.$$
(1.7b)

If the parameter d should be emphasised, we also write $\mathbf{V}_{\text{sym}}^{(d)}$ and $\mathbf{V}_{\text{anti}}^{(d)}$. Correspondingly, if $U \subset V$ is a subspace, the (anti)symmetric tensors in $\otimes^d U$ are denoted by $\mathbf{U}_{\text{sym}}^{(d)}$, resp. $\mathbf{U}_{\text{anti}}^{(d)}$. Another notation for $\mathbf{V}_{\text{anti}}^{(d)}$ is $\bigwedge^d V$ using the exterior product \wedge .

Besides the well-known applications in physics (cf. [2]), symmetric and antisymmetric tensors occur in different mathematical fields.

The symmetric tensor space is related to multivariate polynomials which are homogenous of degree d, i.e., $p(\lambda x) = \lambda^d p(x)$. These polynomials are called *quantics* by Cayley [6]. If $n = \dim(V)$, the symmetric tensor space $\mathbf{V}_{\text{sym}}^{(d)}$ is isomorphic to the vector space of *n*-variate quantics of degree d (cf. [9, §3.5.2]).

The antisymmetric spaces are connected with the Clifford algebra $C\ell_d$ of \mathbb{R}^n , which is isomorphic to the direct sum $\bigoplus_{i=1}^d \bigwedge^j \mathbb{R}^n$ (cf. Lounesto [13, Chap. 22]).

1.1.4 Properties

Since all permutations are products of transpositions $\pi_{i,i+1}$, the next remark follows.

Remark 1.1 A tensor $\mathbf{v} \in \otimes^d V$ is symmetric (resp. antisymmetric) if and only if $\pi(\mathbf{v}) = \pi_{i,i+1}(\mathbf{v})$ (resp. $\pi(\mathbf{v}) = -\pi_{i,i+1}(\mathbf{v})$) holds for all transpositions with $1 \le i < d$.

Let $\mathbf{V} := \otimes^d V$. The linear maps

$$S = S_d := \frac{1}{d!} \sum_{\pi \in \mathbf{P}_d} \pi : \mathbf{V} \to \mathbf{V}, \quad \mathcal{A} = \mathcal{A}_d := \frac{1}{d!} \sum_{\pi \in \mathbf{P}_d} \operatorname{sign}(\pi)\pi : \mathbf{V} \to \mathbf{V}$$
(1.8)

are projections onto \mathbf{V}_{sym} and \mathbf{V}_{anti} , respectively (For a proof note that $\mathcal{S} = \mathcal{S}\pi$ and $\mathcal{A} = \operatorname{sign}(\pi)\mathcal{A}\pi$ so that the application of $\frac{1}{d!}\sum_{\pi \in \mathbf{P}_d}$ yields $\mathcal{S} = \mathcal{S}\mathcal{S}$ and $\mathcal{A} = \mathcal{A}\mathcal{A}$). \mathcal{S} and \mathcal{A} are called the symmetrisation and alternation, respectively.

Remark 1.2 Let $\varphi_{D\setminus\alpha} \in \mathbf{V}'_{D\setminus\alpha}$ be a functional¹ (no symmetry condition assumed). If $\mathbf{v} \in \mathbf{V}^{(D)}_{\text{sym}}$ or $\mathbf{v} \in \mathbf{V}^{(D)}_{\text{anti}}$, then $\varphi_{D\setminus\alpha}(\mathbf{v}) \in \mathbf{V}^{(\alpha)}_{\text{sym}}$ or $\varphi_{D\setminus\alpha}(\mathbf{v}) \in \mathbf{V}^{(\alpha)}_{\text{anti}}$, respectively.

The following expansion lemma will be used in the following.

Lemma 1.3 Let $\{u_1, \ldots, u_r\}$ be a basis of the subspace $U \subset V$. Any tensor $\mathbf{v} \in \otimes^k U$ can be written in the form

$$\mathbf{v} = \sum_{\ell=1}^{r} \mathbf{v}_{[\ell]} \otimes u_{\ell} \qquad \text{with } \mathbf{v}_{[\ell]} \in \otimes^{k-1} U.$$

Let $\{\varphi_1, \ldots, \varphi_r\} \subset U'$ be a dual basis of $\{u_1, \ldots, u_r\}$, i.e., $\varphi_i(u_j) = \delta_{ij}$. Then the tensors $\mathbf{v}_{[\ell]}$ are defined by $\mathbf{v}_{[\ell]} = \varphi_\ell(\mathbf{v})$.

A consequence of the last equation and Remark 1.2 is the following.

Remark 1.4 If $\mathbf{v} \in \otimes^k U$ is (anti-)symmetric, then so is $\mathbf{v}_{[\ell]} \in \otimes^{k-1} U$.

1.2 Minimal Subspaces

Given a tensor $\mathbf{v} \in \mathbf{V} = \bigotimes_{i \in D} V_i$ and a subset $\alpha \subset D$, the corresponding minimal subspace is defined by

$$\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) := \left\{ \varphi_{D \setminus \alpha} \mathbf{v} : \varphi_{D \setminus \alpha} \in \mathbf{V}_{D \setminus \alpha}' \right\} \in \mathbf{V}_{\alpha}$$
(1.9)

(cf. (1.5); [9, §6]). $\mathbf{U}_{\alpha}^{\min}(\mathbf{v})$ is the subspace of smallest dimension with the property $\mathbf{v} \in \mathbf{U}_{\alpha}^{\min}(\mathbf{v}) \otimes \mathbf{V}_{D\setminus\alpha}$. The dual space $\mathbf{V}'_{D\setminus\alpha}$ in (1.9) may be replaced by $\bigotimes_{j \in D\setminus\alpha} V'_j$.

For a subset $\mathbf{V}_0 \subset \mathbf{V}$ we define $\mathbf{U}_{\alpha}^{\min}(\mathbf{V}_0) := \operatorname{span}\{\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) : \mathbf{v} \in \mathbf{V}_0\}.$

Remark 1.5 Let $\emptyset \neq \beta \subsetneq \alpha \subset D$ be nonempty subsets. Then $\mathbf{U}_{\beta}^{\min}(\mathbf{v}) = \mathbf{U}_{\beta}^{\min}(\mathbf{U}_{\alpha}^{\min}(\mathbf{v}))$.

A conclusion from Remark 1.2 is the following statement.

Conclusion 1.6 If $\mathbf{v} \in \mathbf{V}_{sym}$ [or \mathbf{V}_{anti}], then $\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) \subset \mathbf{V}_{sym}^{(\alpha)}$ [or $\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) \subset \mathbf{V}_{anti}^{(\alpha)}$].

¹Compare the definition (1.5) with interchanged subsets α and $D \setminus \alpha$.

2 r-Term Format for (Anti)symmetric Tensors

Let $r \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$. A tensor $\mathbf{v} \in \mathbf{V} = \otimes^d V$ can be represented in the *r*-term format (or canonical format) if there are $v_{\nu}^{(j)} \in V$ for $1 \leq j \leq d$ and $1 \leq \nu \leq r$ such that

$$\mathbf{v} = \sum_{\nu=1}^r \bigotimes_{j=1}^d v_{\nu}^{(j)}.$$

We recall that the smallest possible r in the above representation is called the *rank* of \mathbf{v} and denoted by rank(\mathbf{v}). The number r used above is called the *representation rank*. Since the determination of rank(\mathbf{v}) is NP hard (cf. Håstad [10]) we cannot expect that $r \geq \operatorname{rank}(\mathbf{v})$ holds with an equal sign.

Two approaches to representing (anti)symmetric tensors by the r-term format are described in §2.1 and §2.2.

2.1 Indirect Representation

A symmetric tensor $\mathbf{v} \in \mathbf{V}_{sym}$ may be represented by a general tensor $\mathbf{w} \in \mathbf{V}$ with the property $\mathcal{S}(\mathbf{w}) = \mathbf{v}$, where $\mathcal{S}(\mathcal{A})$ is the symmetrisation (alternation) defined in (1.8). The representation of $\mathbf{w} \in \mathbf{V}$ uses the *r*-term format: $\mathbf{w} = \sum_{i=1}^{r} \bigotimes_{j=1}^{d} w_i^{(j)}$. This approach is proposed by Mohlenkamp, e.g., in [3]. For instance, $\mathbf{v} = a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a \in \mathbf{V}_{sym}$ is represented by $\mathbf{w} = 3a \otimes a \otimes b$. This example indicates that \mathbf{w} may be of a much simpler form than the symmetric tensor $\mathbf{v} = \mathcal{S}(\mathbf{w})$.

However, the cost (storage size) of the representation is only one aspect. Another question concerns the tensor operations. In the following we discuss the addition, the scalar product, and the matrix-vector multiplication.

The *addition* is easy to perform. By linearity of S, the sum of $\mathbf{v}' = S(\mathbf{w}')$ and $\mathbf{v}'' = S(\mathbf{w}'')$ is represented by $\mathbf{w}' + \mathbf{w}''$. Similar in the antisymmetric case.

The summation within the r-term format does not require computational work, but increases the representation rank r. This leads to the question how to truncate $\mathbf{w} = \mathbf{w}' + \mathbf{w}''$ to a smaller rank. It is known that truncation within the r-term format is not an easy task. However, if one succeeds to split \mathbf{w} into $\hat{\mathbf{w}} + \delta \mathbf{w}$, where $\hat{\mathbf{w}}$ has smaller rank and $\delta \mathbf{w}$ is small, this leads to a suitable truncation of $\mathbf{v} = \hat{\mathbf{v}} + \delta \mathbf{v}$ with $\hat{\mathbf{v}} = S(\hat{\mathbf{w}})$, $\delta \mathbf{v} = S(\delta \mathbf{w})$, since $\|\delta \mathbf{v}\| \leq \|\delta \mathbf{w}\|$ with respect to the Euclidean norm.

The computation of the scalar product $\langle \mathbf{v}', \mathbf{v}'' \rangle$ of $\mathbf{v}', \mathbf{v}''$ in \mathbf{V}_{sym} or \mathbf{V}_{anti} is more involved. In the antisymmetric case, $\langle \mathbf{v}', \mathbf{v}'' \rangle$ with $\mathbf{v}' = \mathcal{A}(\mathbf{w}')$, $\mathbf{v}'' = \mathcal{A}(\mathbf{w}'')$ and

$$\mathbf{w}' = \sum_{i'} \bigotimes_{j=1}^{d} w_{i'}^{\prime(j)}, \qquad \mathbf{w}'' = \sum_{i''} \bigotimes_{j=1}^{d} w_{i''}^{\prime\prime(j)}$$

can be written as the sum $\langle \mathbf{v}', \mathbf{v}'' \rangle = \sum_{i', i''} s_{i'i''}$ with the terms

$$s_{i'i''} := \left\langle \mathcal{A}\left(\bigotimes_{j=1}^d w_{i'}^{\prime(j)}\right), \mathcal{A}\left(\bigotimes_{j=1}^d w_{i''}^{\prime\prime(j)}\right) \right\rangle.$$

The latter product coincides with the determinant

$$s_{i'i''} = \det\left(\left(\langle w_{i'}^{\prime(\nu)}, w_{i''}^{\prime\prime(\mu)}\rangle\right)_{1 \le \nu, \mu \le d}\right)$$

(cf. Löwdin [14, (35)]). If the respective representation ranks of \mathbf{v}' and \mathbf{v}'' are r' and r'', the cost amounts to $\mathcal{O}(r'r''d^3)$.

While in the antisymmetric case the determinant can be computed in polynomial time, this does not hold for the analogue in the symmetric case. Instead of the determinant one has to compute the permanent.² As proved by Valiant [17], its computation is NP hard. Hence the computation of the scalar product is only feasible for small d or in special situations.

² The permanent of $A \in \mathbb{R}^{d \times d}$ is $\operatorname{Perm}(A) = \sum_{\pi \in \mathbf{P}_d} \prod_{i=1}^d a_{i,\pi(i)}$.

Next we consider the *multiplication* of a symmetric Kronecker matrix $\mathbf{A} \in \mathbf{L}_{sym} \subset \otimes^d L(V)$ (cf. §9) by a tensor $\mathbf{v} \in \mathbf{V}_{sym/anti} \subset \otimes^d V$. **A** is represented by $\mathbf{B} \in \otimes^d L(V)$ via $\mathbf{A} = \mathcal{S}(\mathbf{B})$ and $\mathbf{B} = \sum_{\nu} \bigotimes_{j=1}^d B_{\nu}^{(j)}$, while $\mathbf{v} = \mathcal{S}(\mathbf{w})$ or $\mathbf{v} = \mathcal{A}(\mathbf{w})$ is represented by $\mathbf{w} = \sum_{\mu} \bigotimes_{j=1}^d w_{\mu}^{(j)}$. The property $\mathbf{v} \in \mathbf{V}_{sym/anti}$ implies the respective property $\mathbf{A} \mathbf{v} \in \mathbf{V}_{sym/anti}$. Unfortunately, $\mathbf{A} \mathbf{v}$ is not the (anti)symmetrisation of $\mathbf{B}\mathbf{w}$. Instead one may use (cf. Lemma 9.1)

$$\mathbf{A} \mathbf{v} = \mathcal{S}(\mathbf{A} \mathbf{w}) = \mathcal{S}(\mathbf{B} \mathbf{v}) \quad \text{or} \quad \mathbf{A} \mathbf{v} = \mathcal{A}(\mathbf{A} \mathbf{w}) = \mathcal{A}(\mathbf{B} \mathbf{v}), \text{ resp.}$$

However, this requires that either the symmetric tensor \mathbf{A} or the (anti)symmetric tensor \mathbf{v} must be constructed explicitly, which contradicts the intention of the indirect representation. Similarly, the Hadamard product $\mathbf{v}' \odot \mathbf{v}''$ and the convolution $\mathbf{v}' \star \mathbf{v}''$ are hard to perform within this format.

Conclusion 2.1 The indirect representation is suited to antisymmetric tensors if only the addition and the scalar product is required. In the case of symmetric tensors, the computation of the scalar product is restricted to small d.

Let $\mathbf{v} \in \mathbf{V}_{\text{sym/anti}}$ be a tensor of rank r_v . The indirect representation uses the r_w -term representation of some $\mathbf{w} \in \mathbf{V}$. The gain is characterised by the ratio r_v/r_w where r_w is the smallest possible rank. According to Seigal [16], the generic reduction factor r_v/r_w is $\frac{(\dim(V)-1)d+1}{\dim(V)}$ which approaches d for large dim(V). The proof uses the results of Abo–Vannieuwenhoven [1]. The conclusion for symmetric tensors is negative: For larger d the computation of the permanent causes difficulties, while for smaller d the gain is only moderate.

2.2 Direct Symmetric *r*-Term Representation

While the previous approach uses general (nonsymmetric) tensors, we now represent the symmetric tensors by an r-term representation involving only symmetric rank-1 tensors:

$$\mathbf{v} = \sum_{i=1}^{r} \alpha_i \otimes^d v_i \quad \text{for suitable } r \in \mathbb{N}_0 \text{ and } v_i \in V, \ \alpha_i \in \mathbb{K}$$
(2.1)

(cf. [9, p. 65]).³ The minimal r in this representation is called the symmetric rank of $\mathbf{v} \in \mathbf{V}_{sym}$ and is denoted by rank_{sym}(\mathbf{v}). Details about symmetric tensors and the symmetric tensor rank are described, e.g., by Comon–Golub–Lim–Mourrain [7].

Since the symmetric rank is at least as large as the standard tensor rank, the required r may be large. A difficulty of the r-term format is caused by the fact that, in general, the set $\{\mathbf{v} \in \otimes^d V : \operatorname{rank}(v) \leq r\}$ is not closed. The simplest counterexamples are symmetric tensors of the form $\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} (\otimes^3 (\mathbf{v} + \varepsilon \mathbf{w}) - \otimes^3 \mathbf{v})$.⁴ Therefore also the subset of the symmetric tensors (2.1) is not closed.

3 Subspace (Tucker) Format

Let $\mathbf{v} \in \mathbf{V}$ be the tensor to be represented. The subspace format (Tucker format) uses subspaces $U_j \subset V_j$ with the property $\mathbf{v} \in \bigotimes_{j=1}^d U_j$. In the (anti)symmetric case one can choose equal subspaces $U \subset V$ (set, e.g., $U = \bigcap_{j=1}^d U_j$). Let $\{u_1, \ldots, u_r\}$ be a basis of U. Then the explicit Tucker representation of \mathbf{v} takes the form

$$\mathbf{v} = \sum_{i_1,\dots,i_d=1}^r c_{i_1,\dots,i_d} \bigotimes_{j=1}^d u_{i_j}$$
(3.1)

with the so-called core tensor $\mathbf{c} \in \bigotimes_{j=1}^{d} \mathbb{K}^{r}$. Obviously, \mathbf{v} is (anti)symmetric if and only if \mathbf{c} is so. Therefore the difficulty is shifted into the treatment of the core tensor. The representation (3.1) itself does not help to represent (anti)symmetric tensors. One may construct hybrid formats, using one of the other representations for \mathbf{c} .

³ If $\mathbb{K} = \mathbb{C}$ or if d is odd, the factor α_i can be avoided since its d-th root can be combined with v_i .

⁴The described limit \mathbf{x} satisfies $\operatorname{rank}_{\operatorname{sym}}(\mathbf{x}) \ge \operatorname{rank}(\mathbf{x}) = d$ (cf. Buczyński–Landsberg [5]), although it is the limit of tensors with symmetric rank 2.

4 Hierarchical Format

In the general case the hierarchical format is a very efficient and flexible representation (cf. [9, §§11–12]). Here we briefly describe the general setting, the TT variant, and first consequences for its application to (anti)symmetric tensors.

4.1 General Case

The recursive partition of the set $D = \{1, \ldots, d\}$ is described by a binary partition tree T_D . It is defined by the following properties: (a) $D \in T_D$ is the root; (b) the singletons $\{1\}, \ldots, \{d\}$ are the leaves; (c) if $\alpha \in T_D$ is not a leaf, the sons $\alpha', \alpha'' \in T_D$ are disjoint sets with $\alpha = \alpha' \cup \alpha''$.

The hierarchical representation of a tensor $v \in \mathbf{V} = \bigotimes_{j=1}^{d} V_j$ is algebraically characterised by subspaces $\mathbf{U}_{\alpha} \subset \mathbf{V}_{\alpha}$ (\mathbf{V}_{α} defined in (1.3)) for all $\alpha \in T_D$ with

$$\mathbf{v} \in \mathbf{U}_D, \tag{4.1a}$$

$$\mathbf{U}_{\alpha} \subset \mathbf{U}_{\alpha'} \otimes \mathbf{U}_{\alpha''} \qquad (\alpha', \alpha'' \text{ sons of } \alpha), \text{ if } \alpha \text{ is not a leaf.}$$
(4.1b)

Let the dimensions of \mathbf{U}_{α} be $r_{\alpha} := \dim(\mathbf{U}_{\alpha})$. Since $\mathbf{U}_{D} = \operatorname{span}(\mathbf{v})$ is sufficient, $r_{D} = 1$ is the general value.

4.2 Implementation

The subspaces \mathbf{U}_{α} are described by bases $\{\mathbf{b}_{k}^{(\alpha)}: k = 1, \ldots, r_{\alpha}\}$. For leaves $\alpha \in T_{D}$, the basis is stored explicitly. Otherwise, condition (4.1b) ensures that

$$\mathbf{b}_{\ell}^{(\alpha)} = \sum_{i=1}^{r_{\alpha'}} \sum_{j=1}^{r_{\alpha''}} c_{ij}^{(\alpha,\ell)} \mathbf{b}_{i}^{(\alpha')} \otimes \mathbf{b}_{j}^{(\alpha'')} \qquad (\alpha', \alpha'' \text{ sons of } \alpha).$$
(4.2)

Therefore it is sufficient to store the coefficients matrices $(c_{ij}^{(\alpha,\ell)})_{1 \leq i \leq r_{\alpha'}, 1 \leq j \leq r_{\alpha''}}$, as well as the vector $c^D \in \mathbb{K}^{r_D}$ for the final representation $\mathbf{v} = \sum_i c_i^D \mathbf{b}_i^{(D)}$ (cf. (4.1a)).

4.3 TT Variant

The TT format is introduced in Oseledets [15] (cf. [9, §12]). It is characterised by a linear tree T_D . That means that the non-leaf vertices $\alpha \in T_D$ are of the form $\alpha = \{1, \ldots, j\}$ with the sons $\alpha' = \{1, \ldots, j-1\}$ and $\alpha'' = \{j\}$. The embedding (4.1b) is $\mathbf{U}_{\{1,\ldots,j+1\}} \subset \mathbf{U}_{\{1,\ldots,j\}} \otimes U_{\{j\}}$.

Below we shall consider the case $\mathbf{V} = \otimes^d V$, i.e., $V_j = V$ is independent of j. Also their subspaces are independent of j and denoted by $U_{\{j\}} = U$. We abbreviate $\mathbf{U}_{\{1,\ldots,j\}}$ by \mathbf{U}_j and denote its dimension by $r_j := \dim(\mathbf{U}_j), r := r_1 = \dim(U)$ (note that $U = \mathbf{U}_1$). Now the nested inclusion (4.1b) becomes

$$\mathbf{U}_{j+1} \subset \mathbf{U}_j \otimes U. \tag{4.3}$$

Similarly, we rewrite $\mathbf{U}_{\{1,\ldots,j\}}^{\min}(\mathbf{v})$ as $\mathbf{U}_{j}^{\min}(\mathbf{v})$.

4.4 (Anti)symmetric Case

Conclusion 1.6 proves that (anti)symmetric tensors \mathbf{v} lead to (anti)symmetric minimal subspaces: $\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) \subset \mathbf{V}_{\text{sym}}^{(\alpha)}$ or $\mathbf{U}_{\alpha}^{\min}(\mathbf{v}) \in \mathbf{V}_{\text{anti}}^{(\alpha)}$, respectively.

The hierarchical representation (4.1a,b) of $\mathbf{v} \in \mathbf{V}_{sym}^{(D)}$ should also use subspaces with the property $\mathbf{U}_{\alpha} \subset \mathbf{V}_{sym}^{(\alpha)}$ (similar in the antisymmetric case).

The basic task is the determination of a basis $\mathbf{b}_{\ell}^{(\alpha)} \in \mathbf{U}_{\alpha} \subset \mathbf{V}_{\text{sym}}^{(\alpha)}$ $(1 \leq \ell \leq r_{\alpha} := \dim(\mathbf{U}_{\alpha}))$ by suitable linear combinations of the tensors $\mathbf{b}_{i}^{(\alpha')} \otimes \mathbf{b}_{j}^{(\alpha'')}$. The assumptions $\mathbf{b}_{i}^{(\alpha')} \in \mathbf{V}_{\text{sym}}^{(\alpha')}$ and $\mathbf{b}_{j}^{(\alpha'')} \in \mathbf{V}_{\text{sym}}^{(\alpha'')}$ lead to a partial symmetry, but, in general, $\pi_{\nu\mu}(\mathbf{b}_{\ell}^{(\alpha)}) = \mathbf{b}_{\ell}^{(\alpha)}$ is not satisfied for $\nu \in \alpha'$ and $\mu \in \alpha''$.

Using (4.3) and symmetry, we conclude that

$$\mathbf{U}_j \subset \left(\otimes^j U\right) \cap \mathbf{V}_{\text{sym}}^{(j)} = \mathbf{U}_{\text{sym}}^{(j)}.$$
(4.4)

Remark 4.1 (a) Because of (4.4) we can restrict the vector space V in (1.7a,b) to U. (b) If we want to represent the tensor \mathbf{v} , the subspace \mathbf{U}_j must satisfy

$$\mathbf{U}_{i}^{\min}(\mathbf{v}) \subset \mathbf{U}_{i}.$$

4.5 Dimensions of U_i^{\min} in the (Anti)symmetric Case

The following statement shows that, in the case of antisymmetric tensors, the hierarchical approach becomes costly for high dimensions d. The simplest antisymmetric tensor is the antisymmetrisation of an elementary tensor:

$$\mathbf{a} := \mathcal{A}\left(\bigotimes_{j=1}^{d} u^{(j)}\right).$$

To ensure $\mathbf{a} \neq 0$, the vectors $u^{(j)}$ must be linearly independent. In that case the minimal subspace $\mathbf{U}_k^{\min}(\mathbf{v})$ is spanned by all tensors $\mathcal{A}\left(\bigotimes_{j=1}^k u^{(i_j)}\right)$ with $1 \leq i_1 < i_2 < \ldots < i_k \leq d$. There are $\binom{k}{d}$ tensors of this form. Since they are linearly independent, dim $\mathbf{U}_k^{\min}(\mathbf{a}) = \binom{k}{d}$ follows. The sum $\sum_{k=1}^d \dim \mathbf{U}_k^{\min}(\mathbf{a})$ is $2^d - 1$. Hence, this approach cannot be recommended for large d.

The situation is different in the symmetric case, since the vectors in $\mathcal{S}(\bigotimes_{j=1}^{d} u^{(j)})$ need not be linearly independent. The next lemma uses the symmetric rank defined in §2.2.

Lemma 4.2 All symmetric tensors \mathbf{v} satisfy dim $\mathbf{U}_k^{\min}(\mathbf{v}) \leq \operatorname{rank}_{\operatorname{sym}}(\mathbf{v})$.

Proof. Let $\mathbf{v} = \sum_{i=1}^{r} \alpha_i \otimes^d v_i$ with $r = \operatorname{rank_{sym}}(\mathbf{v})$. Then all minimal subspaces $\mathbf{U}_k^{\min}(\mathbf{v})$ are contained in the *r*-dimensional space span $\{\otimes^k v_i : 1 \le i \le r\}$.

The following symmetric tensor describes, e.g., the structure of the Laplace operator (a, b) of the next example are the identity map and one-dimensional Laplacian, respectively).

Example 4.3 An important example is the symmetric tensor $\mathbf{v} := \mathcal{S}(\otimes^{d-1} a \otimes b)$, where $a, b \in V$ are linearly independent. In this case we have

 $\dim(\mathbf{U}_k^{\min}(\mathbf{v})) = 2 \qquad for \ 1 \le k < d.$

More precisely, $\mathbf{U}_k^{\min}(\mathbf{v})$ is spanned by $\otimes^k a$ and $\mathcal{S}_k(b \otimes (\otimes^{k-1} a))$.

5 TT Format for Symmetric Tensors

In the following we focus on the representation of symmetric tensors in the TT format (cf. $\S4.3$). In principle, the same technique can be used for antisymmetric tensors (but compare $\S4.5$).

In §5.4 we try to construct the space \mathbf{U}_{j+1} from \mathbf{U}_j . This will lead to open questions in §5.4.6. If we start from \mathbf{v} and the related minimal subspace $\mathbf{U}_j^{\min}(\mathbf{v})$, then an appropriate choice is $\mathbf{U}_j = \mathbf{U}_j^{\min}(\mathbf{v})$ (see §5.5).

5.1 The Space $(\mathbf{U}_j \otimes U) \cap \mathcal{S}(\mathbf{U}_j \otimes U)$ and the Principal Idea

We want to repeat the same construction of nested spaces as in (4.3). In contrast to the general case, we also have to ensure symmetry. By induction, we assume that \mathbf{U}_j contains only symmetric tensors:

$$\mathbf{U}_j \subset \mathbf{V}_{\rm sym}^{(j)}.\tag{5.1}$$

On the one hand, the new space \mathbf{U}_{j+1} should satisfy $\mathbf{U}_{j+1} \subset \mathbf{U}_j \otimes U$; on the other hand, symmetry $\mathbf{U}_{j+1} \subset \mathbf{V}_{sym}^{(j+1)}$ is required. Together, $\mathbf{U}_{j+1} \subset (\mathbf{U}_j \otimes U) \cap \mathbf{V}_{sym}^{(j+1)}$ must be ensured.

Remark 5.1 $(\mathbf{U}_j \otimes U) \cap \mathbf{V}_{\text{sym}}^{(j+1)} = (\mathbf{U}_j \otimes U) \cap \mathcal{S}_{j+1} (\mathbf{U}_j \otimes U)$ holds with the symmetrisation \mathcal{S}_{j+1} in (1.8).

Proof. Let $\mathbf{v} \in (\mathbf{U}_j \otimes U) \cap \mathbf{V}_{\text{sym}}^{(j+1)}$. Since $\mathbf{v} \in \mathbf{V}_{\text{sym}}^{(j+1)}$, $\mathcal{S}(\mathbf{v}) = \mathbf{v}$ holds. Since $\mathbf{v} \in \mathbf{U}_j \otimes U$, $\mathbf{v} = \mathcal{S}(\mathbf{v}) \in \mathcal{S}(\mathbf{U}_j \otimes U)$ follows. This proves $(\mathbf{U}_j \otimes U) \cap \mathbf{V}_{\text{sym}}^{(j+1)} \subset (\mathbf{U}_j \otimes U) \cap \mathcal{S}(\mathbf{U}_j \otimes U)$. The reverse inclusion follows from $\mathcal{S}(\mathbf{U}_j \otimes U) \subset \mathbf{V}_{\text{sym}}^{(j+1)}$.

This leads us to the condition

$$\mathbf{U}_{j+1} \subset \hat{\mathbf{U}}_{j+1} := (\mathbf{U}_j \otimes U) \cap \mathcal{S}(\mathbf{U}_j \otimes U)$$
(5.2)

for the choice of the next subspace \mathbf{U}_{j+1} .

It must be emphasised that, in general, $\mathcal{S}(\mathbf{U}_j \otimes U)$ is not a subspace of $\mathbf{U}_j \otimes U$. Example 5.14 will show nontrivial subspaces \mathbf{U}_j, U that may even lead to $\hat{\mathbf{U}}_{j+1} = \{0\}$.

To repeat the construction (4.2), we assume that there is a basis $\{\mathbf{b}_1^{(j)}, \ldots, \mathbf{b}_{r_j}^{(j)}\}$ of \mathbf{U}_j and the basis $\{u_1, \ldots, u_r\}$ of U. Then the basis $\{\mathbf{b}_1^{(j+1)}, \ldots, \mathbf{b}_{r_{j+1}}^{(j+1)}\}$ of \mathbf{U}_{j+1} can be constructed by (4.2) which now takes the form

$$\mathbf{b}_{k}^{(j+1)} = \sum_{\nu=1}^{r_{j}} \sum_{\mu=1}^{r} c_{\nu\mu}^{(k)} \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu} \qquad (1 \le k \le r_{j+1}).$$
(5.3)

In order to check linear independence and to construct orthonormal bases, we also have to require that we are able to determine scalar products. Assuming by induction that the scalar products $\langle \mathbf{b}_{\nu'}^{(j)}, \mathbf{b}_{\nu''}^{(j)} \rangle$ and $\langle u_{\mu'}, u_{\mu''} \rangle$ are known, the value of $\langle \mathbf{b}_{k'}^{(j+1)}, \mathbf{b}_{k''}^{(j+1)} \rangle$ follows from (1.4). Therefore, we are able to form an orthonormal basis of \mathbf{U}_{j+1} .

To avoid difficulties with a too small intersection $\hat{\mathbf{U}}_{j+1}$, an alternative idea could be to choose the subspace \mathbf{U}_{j+1} in $\mathcal{S}(\mathbf{U}_j \otimes U)$ and not necessarily in $\mathbf{U}_j \otimes U$. Then, instead of (5.3), we have $\mathbf{b}_k^{(j+1)} = \sum_{\nu,\mu} c_{\nu\mu}^{(k)} \mathcal{S}(\mathbf{b}_{\nu}^{(j)} \otimes u_{\mu})$. This would be a very flexible approach, were it not for the fact that we need knowledge of the scalar products $\left\langle s_{\nu\mu}^{(j)}, s_{\nu'\mu'}^{(j)} \right\rangle$ for $s_{\nu\mu}^{(j)} := \mathcal{S}(\mathbf{b}_{\nu}^{(j)} \otimes u_{\mu})$ (otherwise, an orthonormal basis $\{\mathbf{b}_k^{(j+1)}\}$ cannot be constructed). One finds that

$$\left\langle s_{\nu\mu}^{(j)}, s_{\nu'\mu'}^{(j)} \right\rangle = \frac{\delta_{\mu\mu'}}{j+1} \left\langle \mathbf{b}_{\nu}^{(j)}, \mathbf{b}_{\nu'}^{(j)} \right\rangle + \frac{j}{j+1} \left\langle \mathbf{b}_{\nu,[\mu']}^{(j)}, \mathbf{b}_{\nu',[\mu]}^{(j)} \right\rangle$$

where the expression $\mathbf{b}_{\nu,[\mu']}^{(j)}$ is defined in Lemma 1.3. The scalar products $\left\langle \mathbf{b}_{\nu,[\mu']}^{(j)}, \mathbf{b}_{\nu',[\mu]}^{(j)} \right\rangle$ can be derived from $\left\langle s_{\nu\mu,[\ell]}^{(j)}, s_{\nu'\mu',[\ell']}^{(j)} \right\rangle$. This expression, however, requires the knowledge of $\left\langle \mathbf{b}_{\nu,[\ell,\mu']}^{(j-1)}, \mathbf{b}_{\nu',[\ell',\mu]}^{(j-1)} \right\rangle$ (concerning the subscript $[\ell,\mu']$ compare (5.7)). Finally, we need scalar products of the systems $\{\mathbf{b}_{\nu}^{(d)}\}, \{\mathbf{b}_{\nu}^{(d-1)}\}, \{\mathbf{b}_{\nu,[\mu]}^{(d-1)}\}, \{\mathbf{b}_{\nu,[\mu]}^{(d-2)}\}, \dots, \{\mathbf{b}_{\nu,[\ell_1,\ell_2,\dots,\ell_{j^*}]}^{(j)}\}$ with $j^* = \min\{j, d-j\}, \dots$. This leads to a data size increasing exponentially in d.

5.2 The Spaces $(\mathbf{U}_{j} \otimes U) \cap \mathcal{S}(\mathbf{U}_{j} \otimes U)$ and $\mathbf{U}_{i+1}^{\min}(\mathbf{v})$

Let $\mathbf{v} \in (\otimes^d V) \cap \mathbf{V}_{sym}^{(d)}$ be the symmetric tensor which we want to represent. We recall the minimal subspaces defined in §1.2. According to the notation of the TT format, $\mathbf{U}_j^{\min}(\mathbf{v})$ is the space $\mathbf{U}_{\{1,\dots,j\}}^{\min}(\mathbf{v}) \subset \otimes^j V$ defined in (1.9). The minimality property of $\mathbf{U}_j^{\min}(\mathbf{v})$ (cf. [9, §6]) implies that the subspaces U and \mathbf{U}_j must satisfy

$$U \supset U_1^{\min}(\mathbf{v}), \qquad \mathbf{U}_j \supset \mathbf{U}_j^{\min}(\mathbf{v});$$
 (5.4)

otherwise \mathbf{v} cannot be represented by the TT format.

The next theorem states that (5.4) guarantees that there is a suitable subspace \mathbf{U}_j with $\hat{\mathbf{U}}_j \supset \mathbf{U}_j \supset \mathbf{U}_j$ $\mathbf{U}_j^{\min}(\mathbf{v})$, so that the requirement (5.4) is also valid for j + 1.

Theorem 5.2 Let (5.4) be valid for $\mathbf{v} \in \mathbf{U}_{sym}^{(d)}$ and let j < d. Then $\hat{\mathbf{U}}_{j+1}$ in (5.2) satisfies $\hat{\mathbf{U}}_{j+1} \supset \mathbf{U}_{j+1}^{\min}(\mathbf{v})$.

Proof. We have $\mathbf{U}_j \otimes U \supset \mathbf{U}_j^{\min}(\mathbf{v}) \otimes U_1^{\min}(\mathbf{v})$. A general property of the minimal subspace is

$$\mathbf{U}_{i}^{\min}(\mathbf{v}) \otimes U_{1}^{\min}(\mathbf{v}) \supset \mathbf{U}_{i+1}^{\min}(\mathbf{v})$$

(cf. [9, Proposition 6.17]). Since $\mathbf{U}_{i+1}^{\min}(\mathbf{v})$ is symmetric (cf. Conclusion 1.6), it follows that

$$\mathcal{S}(\mathbf{U}_{j} \otimes U) \supset \mathcal{S}(\mathbf{U}_{j}^{\min}(\mathbf{v}) \otimes U_{1}^{\min}(\mathbf{v})) \supset \mathcal{S}(\mathbf{U}_{j+1}^{\min}(\mathbf{v})) = \mathbf{U}_{j+1}^{\min}(\mathbf{v}).$$

This inclusion together with the previous inclusion $\mathbf{U}_j \otimes U \supset \mathbf{U}_{j+1}^{\min}(\mathbf{v})$ yields the statement.

So far, we could ensure that there exists a suitable subspace $\mathbf{U}_{j+1} \supset \mathbf{U}_{j+1}^{\min}(\mathbf{v})$. Concerning the practical implementation, two questions remain:

(a) How can we find the subspace $\hat{\mathbf{U}}_{j+1} \subset \mathbf{U}_j \otimes U$?

(b) Given $\hat{\mathbf{U}}_{j+1}$, how can we ensure $\mathbf{U}_{j+1} \supset \mathbf{U}_{j+1}^{\min}(\mathbf{v})$?

The next subsection yields a partial answer to the first question.

5.3 Criterion for Symmetry

According to Lemma 1.3, any $\mathbf{v} \in \mathbf{U}_j \otimes U$ is of the form

$$\mathbf{v} = \sum_{\ell=1}^{j} \mathbf{v}_{[\ell]} \otimes u_{\ell} \qquad (\mathbf{v}_{[\ell]} \in \mathbf{U}_j).$$
(5.5)

The mapping $\mathbf{v} \in \mathbf{V}^{(j+1)} \mapsto \mathbf{v}_{[\ell]} \in \mathbf{V}^{(j)}$ can be iterated:

$$\mathbf{v}_{[\ell]} \in \mathbf{V}^{(j)} \mapsto (\mathbf{v}_{[\ell]})_{[m]} = \mathbf{v}_{[\ell][m]} = \mathbf{v}_{[\ell,m]} \in \mathbf{V}^{(j-1)}$$

In the case of j = 1, the empty product $\otimes^{j-1} V$ is defined as the field \mathbb{K} , i.e., $\mathbf{v}_{[\ell,m]}$ is a scalar.

Lemma 5.3 A necessary and sufficient condition for $\mathbf{v} \in \mathbf{V}_{sym}^{(j+1)}$ is

$$\mathbf{v}_{[\ell]} \in \mathbf{V}_{\text{sym}}^{(j)} \quad and \quad \mathbf{v}_{[\ell,m]} = \mathbf{v}_{[m,\ell]} \quad for \ all \ 1 \le \ell, m \le r.$$
(5.6)

Here, $\mathbf{v}_{[\ell]}$ refers to (5.5), and $\mathbf{v}_{[\ell,m]}$ is the expansion term of $\mathbf{v}_{[\ell]} \in \bigotimes^j V$.

Proof. (a) Assume $\mathbf{v} \in \mathbf{V}_{\text{sym}}^{(j+1)}$. $\mathbf{v}_{[\ell]} \in \mathbf{V}_{\text{sym}}^{(j)}$ is stated in Remark 1.4. Applying the expansion to $\mathbf{v}_{[\ell]}$ in (5.5), we obtain

$$\mathbf{v} = \sum_{\ell,m=1}^{r} \mathbf{v}_{[\ell,m]} \otimes u_m \otimes u_\ell.$$
(5.7)

Note that the tensors $\{u_m \otimes u_\ell : 1 \leq \ell, m \leq r\}$ are linearly independent. Therefore, transposition $u_m \otimes u_\ell \mapsto u_\ell \otimes u_m$ and symmetry of **v** imply that $\mathbf{v}_{[\ell,m]} = \mathbf{v}_{[m,\ell]}$.

(b) Assume (5.6). Because of $\mathbf{v}_{[\ell]} \in \mathbf{V}_{\text{sym}}^{(j)}$, \mathbf{v} is invariant under all transpositions $\pi_{i,i+1}$ for $1 \leq i < j$. Condition $\mathbf{v}_{[\ell,m]} = \mathbf{v}_{[m,\ell]}$ ensures that \mathbf{v} is also invariant under the transposition $\pi_{j,j+1}$. This proves the symmetry of \mathbf{v} (cf. Remark 1.1).

To apply this criterion to the construction of $\hat{\mathbf{U}}_{j+1} := (\mathbf{U}_j \otimes U) \cap \mathcal{S}(\mathbf{U}_j \otimes U)$, we search for a symmetric tensor (5.3) of the form

$$\mathbf{b} = \sum_{\nu=1}^{r_j} \sum_{\mu=1}^r c_{\nu\mu} \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu}.$$
(5.8)

The tensor **b** corresponds to $\mathbf{v}_{[\ell]} := \sum_{\nu=1}^{r_j} c_{\nu\ell} \mathbf{b}_{\nu}^{(j)}$ in (5.5). $\mathbf{v}_{[\ell]} \in \mathbf{V}_{\text{sym}}^{(j)}$ is satisfied because of (5.1). The condition $\mathbf{v}_{[\ell,m]} = \mathbf{v}_{[m,\ell]}$ in (5.6) becomes

$$\sum_{\nu=1}^{r_j} c_{\nu\ell} \mathbf{b}_{\nu,[m]}^{(j)} = \sum_{\nu=1}^{r_j} c_{\nu m} \mathbf{b}_{\nu,[\ell]}^{(j)}.$$
(5.9)

The tensors $\mathbf{b}_{\nu,[m]}^{(j)}$ and $\mathbf{b}_{\nu,[\ell]}^{(j)}$ belong to \mathbf{U}_{j-1} . The new (nontrivial) algebraic task is to find the set of coefficients $c_{\nu\mu}$ satisfying (5.9) for all $1 \leq \ell, m \leq r$.

Remark 5.4 The ansatz (5.8) has $rr_j - 1$ free parameters (one has to be subtracted because of the normalisation). Condition (5.9) describes $\frac{r(r-1)}{2}$ equations in the space \mathbf{U}_{j-1} equivalent to $\frac{r(r-1)}{2}r_{j-1}$ scalar equations.

5.4 TT Symmetrisation

In the following approach we obtain a symmetric tensor in $\mathcal{S}(\mathbf{U}_i \otimes U)$, but not necessarily in $\mathbf{U}_i \otimes U$.

5.4.1 Symmetrisation Operator S_{j+1}

In the present approach we directly symmetrise the tensors. The general symmetrisation map S consists of d! terms. However, since \mathbf{U}_j is already symmetric, tensors in $\mathbf{U}_j \otimes U$ can be symmetrised by only j + 1transpositions $\pi_{i,j+1}$.

Theorem 5.5 Let $\mathbf{v}^{(j)} \in \mathbf{V}_{sym}^{(j)}$ and $w \in V$. Applying

$$\hat{\mathcal{S}}_{j+1} := \frac{1}{j+1} \sum_{i=1}^{j+1} \pi_{i,j+1}$$

to $\mathbf{v}^{(j)} \otimes w \in \mathbf{V}^{(j+1)}$ yields a symmetric tensor:

$$\mathbf{s} := \hat{\mathcal{S}}_{j+1} \left(\mathbf{v}^{(j)} \otimes w \right) \in \mathbf{V}_{\mathrm{sym}}^{(j+1)}.$$

Proof. According to Remark 1.1, we have to show that $\pi_{k,k+1}\mathbf{s} = \mathbf{s}$ for all $1 \le k \le j$. First we consider the case of k < j. If $i \notin \{k, k+1\}$, we have $\pi_{k,k+1}\pi_{i,j+1} = \pi_{i,j+1}\pi_{k,k+1}$. For $i \in \{k, k+1\}$ we obtain

$$\pi_{k,k+1}\pi_{k,j+1} = \pi_{k+1,j+1}\pi_{k,k+1}, \qquad \pi_{k,k+1}\pi_{k+1,j+1} = \pi_{k,j+1}\pi_{k,k+1}.$$

This proves $\pi_{k,k+1}\hat{\mathcal{S}}_{j+1} = \hat{\mathcal{S}}_{j+1}\pi_{k,k+1}$ and

$$\pi_{k,k+1}\mathbf{s} = \hat{\mathcal{S}}_{j+1}\pi_{k,k+1}\left(\mathbf{v}^{(j)}\otimes w\right) = \hat{\mathcal{S}}_{j+1}\left(\pi_{k,k+1}\mathbf{v}^{(j)}\otimes w\right).$$

Symmetry of $\mathbf{v}^{(j)}$ implies $\pi_{k,k+1}\mathbf{v}^{(j)} = \mathbf{v}^{(j)}$ so that $\pi_{k,k+1}\mathbf{s} = \mathbf{s}$ is proved.

The remaining case is k = j. For i < j, the identity $\pi_{j,j+1}\pi_{i,j+1} = \pi_{i,j+1}\pi_{i,j}$ together with $\pi_{i,j}\mathbf{v}^{(j)} = \mathbf{v}^{(j)}$ implies $\pi_{j,j+1}\pi_{i,j+1}(\mathbf{v}^{(j)} \otimes w) = \pi_{i,j+1}(\mathbf{v}^{(j)} \otimes w)$. For $i \in \{j, j+1\}$ we obtain

$$\pi_{j,j+1}\pi_{j,j+1} = \mathrm{id} = \pi_{j+1,j+1}, \qquad \pi_{j,j+1}\pi_{j+1,j+1} = \pi_{j,j+1} \cdot \mathrm{id} = \pi_{j,j+1};$$

i.e., $\pi_{j,j+1} (\pi_{i,j+1} + \pi_{j+1,j+1}) = \pi_{i,j+1} + \pi_{j+1,j+1}$. Hence, also $\pi_{j,j+1} \mathbf{s} = \mathbf{s}$ is proved.

Corollary 5.6 The corresponding antisymmetrisation is obtained by

$$\hat{\mathcal{A}}_d := \frac{1}{d} \sum_{i=1}^d (-1)^{d-i} \pi_{id}.$$

Although the symmetrisation ensures that $\mathbf{s} \in \mathcal{S}(\mathbf{U}_j \otimes U)$, there is no guaranty that $\mathbf{s} \in \mathbf{U}_j \otimes U$. Hence, whether $\mathbf{s} \in \hat{\mathbf{U}}_{j+1}$ holds or not is still open.

5.4.2 Expansion of s

Since $\mathbf{v}^{(j)} \otimes w \in \otimes^{j+1} U$, the symmetrisation $\mathbf{s} = \hat{\mathcal{S}}_{j+1}(\mathbf{v}^{(j)} \otimes w)$ also belongs to $\otimes^{j+1} U$. By Lemma 1.3 there is a representation $\mathbf{s} = \sum_{\ell=1}^{r} \mathbf{s}_{[\ell]} \otimes u_{\ell}$ with $\mathbf{s}_{[\ell]} \in \mathbf{U}_{\text{sym}}^{(j)}$.

Lemma 5.7 Let $w = \sum_{\ell=1}^{r} c_{\ell} u_{\ell}$ and $\mathbf{v}^{(j)} \in \mathbf{U}_{sym}^{(j)}$. Then $\mathbf{s} := \hat{\mathcal{S}}_{j+1}(\mathbf{v}^{(j)} \otimes w)$ satisfies

$$\mathbf{s} = \sum_{\ell=1}^{r} \mathbf{s}_{[\ell]} \otimes u_{\ell} \quad with \ \mathbf{s}_{[\ell]} := \frac{1}{j+1} \left(c_{\ell} \mathbf{v}^{(j)} + \sum_{i=1}^{j} \pi_{i,j} \left(\mathbf{v}_{[\ell]}^{(j)} \otimes w \right) \right).$$
(5.10)

The latter sum $\sum_{i=1}^{j} \pi_{i,j}(\mathbf{v}_{[\ell]}^{(j)} \otimes w)$ can be written as $j\hat{\mathcal{S}}_{j}(\mathbf{v}_{[\ell]}^{(j)} \otimes w)$.

Proof. Using $\pi_{j+1,j+1} = id$, we obtain

$$(j+1)\mathbf{s} = \mathbf{v}^{(j)} \otimes w + \sum_{i=1}^{j} \pi_{i,j+1}(\mathbf{v}^{(j)} \otimes w) = \sum_{\ell=1}^{r} c_{\ell} \mathbf{v}^{(j)} \otimes u_{\ell} + \sum_{i=1}^{j} \pi_{i,j+1}(\mathbf{v}^{(j)} \otimes w).$$

Since $\pi_{i,j+1} = \pi_{i,j}\pi_{j,j+1}\pi_{i,j}$ for $i \leq j$ and $\mathbf{v}^{(j)} = \sum_{\ell=1}^{r} \mathbf{v}_{[\ell]}^{(j)} \otimes u_{\ell} \in \mathbf{U}_{\text{sym}}^{(j)}$, we have

$$\pi_{i,j+1}(\mathbf{v}^{(j)} \otimes w) = \pi_{i,j}\pi_{j,j+1}\left((\pi_{i,j}\mathbf{v}^{(j)}) \otimes w\right) = \pi_{i,j}\pi_{j,j+1}\left(\mathbf{v}^{(j)} \otimes w\right)$$
$$= \pi_{i,j}\pi_{j,j+1}\sum_{\ell=1}^{r}\mathbf{v}_{[\ell]}^{(j)} \otimes u_{\ell} \otimes w = \pi_{i,j}\sum_{\ell=1}^{r}\mathbf{v}_{[\ell]}^{(j)} \otimes w \otimes u_{\ell} = \sum_{\ell=1}^{r}\left(\pi_{i,j}(\mathbf{v}_{[\ell]}^{(j)} \otimes w)\right) \otimes u_{\ell}.$$

Together we obtain (j+1) $\mathbf{s} = \sum_{\ell=1}^{r} \left(c_{\ell} \mathbf{v}^{(j)} + \sum_{\ell=1}^{r} \left(\pi_{i,j} (\mathbf{v}_{[\ell]}^{(j)} \otimes w) \right) \right) \otimes u_{\ell}.$

The last equation explicitly provides the expansion of ${\bf s}$ defined in Lemma 1.3.

5.4.3 Scalar Products

The definition of $\mathbf{s} := \hat{\mathcal{S}}_{j+1}(\mathbf{v}^{(j)} \otimes w)$ seems a bit abstract, since (5.10) contains the permuted tensor which not necessarily belongs to $\mathbf{U}_j \otimes U$. Even in that case it is possible to determine the scalar products $\langle \mathbf{s}, \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu} \rangle$ with the basis vectors $\mathbf{b}_{\nu}^{(j)} \otimes u_{\mu}$ of $\mathbf{U}_j \otimes U$. The first term in (5.10) yields

$$\left\langle \mathbf{v}^{(j)} \otimes u_{\ell}, \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu} \right\rangle = \left\langle \mathbf{v}^{(j)}, \mathbf{b}_{\nu}^{(j)} \right\rangle \left\langle u_{\ell}, u_{\mu} \right\rangle$$

By induction, we assume that the scalar product of $\mathbf{v}^{(j)} \in \mathbf{U}_j$ and $\mathbf{b}^{(j)}_{\nu}$ is known. Usually, the basis $\{u_\ell\}$ is chosen orthonormal so that $\langle u_\ell, u_\mu \rangle = \delta_{\ell\mu}$. The other terms yield the products

$$\left\langle \pi_{i,j}\left(\mathbf{v}_{[\ell]}^{(j)} \otimes w \otimes u_{\ell}\right), \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu} \right\rangle = \left\langle \pi_{i,j}\left(\mathbf{v}_{[\ell]}^{(j)} \otimes w\right), \mathbf{b}_{\nu}^{(j)} \right\rangle \left\langle u_{\ell}, u_{\mu} \right\rangle.$$

Using the selfadjointness of $\pi_{i,j}$ and $\mathbf{b}_{\nu}^{(j)} \in \mathbf{V}_{sym}^{(j)}$, we obtain

$$\left\langle \pi_{i,j} \left(\mathbf{v}_{[\ell]}^{(j)} \otimes w \right), \mathbf{b}_{\nu}^{(j)} \right\rangle = \left\langle \mathbf{v}_{[\ell]}^{(j)} \otimes w, \pi_{i,j} \mathbf{b}_{\nu}^{(j)} \right\rangle = \left\langle \mathbf{v}_{[\ell]}^{(j)} \otimes w, \mathbf{b}_{\nu}^{(j)} \right\rangle$$
$$= \left\langle \mathbf{v}_{[\ell]}^{(j)} \otimes w, \sum_{k=1}^{r} \mathbf{b}_{\nu,[k]}^{(j)} \otimes u_{k} \right\rangle = \sum_{k=1}^{r} \left\langle \mathbf{v}_{[\ell]}^{(j)}, \mathbf{b}_{\nu,[k]}^{(j)} \right\rangle \langle w, u_{k} \rangle$$

If $\{u_\ell\}$ is an orthogonal basis, $\langle w, u_k \rangle = c_k$ holds (cf. Lemma 5.7).

Remark 5.8 Let the bases $\{\mathbf{b}_{\nu}^{(j)} : 1 \leq \nu \leq r_j\}$ and $\{u_{\ell} : 1 \leq \ell \leq r\}$ be orthonormal. If $\mathbf{s} := \hat{\mathcal{S}}_{j+1}(\mathbf{v}^{(j)} \otimes w) \in \mathbf{U}_j \otimes U$, the explicit representation is given by

$$\mathbf{s} = \sum_{\nu=1}^{r_j} \sum_{\mu=1}^r c_{\nu\mu} \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu}$$
(5.11)

with coefficients $c_{\nu\mu} = \langle \mathbf{s}, \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu} \rangle$, which are computable as explained above.

Even if $\mathbf{s} \notin \mathbf{U}_j \otimes U$, the right-hand side in (5.11) is computable and describes the orthogonal projection $P_{\mathbf{U}_j \otimes U}\mathbf{s}$ of \mathbf{s} onto the space $\mathbf{U}_j \otimes U$.

The check whether **s** belongs to $\mathbf{U}_j \otimes U$ is equivalent to the check whether $P_{\mathbf{U}_j \otimes U}\mathbf{s}$ is symmetric (cf. §5.3), as stated next.

Criterion 5.9 $\mathbf{s} \in \mathbf{U}_j \otimes U$ [and therefore also $\mathbf{s} \in \hat{\mathbf{U}}_{j+1}$, cf. (5.2)] holds if and only if $P_{\mathbf{U}_j \otimes U}\mathbf{s} = \mathbf{s} \in \mathbf{V}_{\text{sym}}^{(j+1)}$ (implying $P_{\mathbf{U}_j \otimes U}\mathbf{s} \in \hat{\mathbf{U}}_{j+1}$ in the positive case).

Proof. (a) Abbreviate $P_{\mathbf{U}_j \otimes U}$ by P. Let $\mathbf{s} \in \mathbf{U}_j \otimes U$. This implies $P\mathbf{s} = \mathbf{s}$. Since, by construction, \mathbf{s} is symmetric, $P\mathbf{s} \in \mathbf{V}_{sym}^{(j+1)}$ holds.

(b) Assume $P\mathbf{s} \in \mathbf{V}_{\text{sym}}^{(j+1)}$. Because of $\mathbf{s} = P\mathbf{s} + (I - P)\mathbf{s}$, also $\mathbf{s}^{\perp} := (I - P)\mathbf{s} \in (\mathbf{U}_j \otimes U)^{\perp}$ is symmetric. The properties of projections show

$$\langle \mathbf{s}^{\perp}, \mathbf{s}^{\perp} \rangle = \langle (I-P)\mathbf{s}, (I-P)\mathbf{s} \rangle = \langle \mathbf{s}, (I-P)\mathbf{s} \rangle = \langle \mathcal{S}_{j+1}(\mathbf{v}^{(j)} \otimes w), \mathbf{s}^{\perp} \rangle.$$

Since S_{j+1} is selfadjoint and \mathbf{s}^{\perp} is symmetric, we have

$$\langle \mathbf{s}^{\perp}, \mathbf{s}^{\perp} \rangle = \langle \mathbf{v}^{(j)} \otimes w, \mathcal{S}_{j+1} \mathbf{s}^{\perp} \rangle = \langle \mathbf{v}^{(j)} \otimes w, \mathbf{s}^{\perp} \rangle = 0$$

because of $\mathbf{v}^{(j)} \otimes w \in \mathbf{U}_j \otimes U$ and $\mathbf{s}^{\perp} \in (\mathbf{U}_j \otimes U)^{\perp}$. This proves $\mathbf{s}^{\perp} = 0$ and $\mathbf{s} = P_{\mathbf{U}_j \otimes U}\mathbf{s}$, i.e., $\mathbf{s} \in \mathbf{U}_j \otimes U$.

5.4.4 Geometric Characterisation

Let $\{\mathbf{b}_{\nu}^{(j)}: 1 \leq \nu \leq r_j\}$ and $\{u_{\mu}: 1 \leq \mu \leq r\}$ be orthonormal bases of $\mathbf{U}_j \subset \mathbf{U}_{\text{sym}}^{(j)}$ and U, respectively. $\mathbf{b}_{\nu,[\ell]}^{(j)}$ are the expansion terms: $\mathbf{b}_{\nu}^{(j)} = \sum_{\ell} \mathbf{b}_{\nu,[\ell]}^{(j)} \otimes u_{\ell}$. They give rise to the scalar products

$$B_{(\nu,\mu),(\nu',\mu')} := \left\langle \mathbf{b}_{\nu,[\mu']}^{(j)}, \mathbf{b}_{\nu',[\mu]}^{(j)} \right\rangle \qquad (1 \le \nu, \nu' \le r_j, 1 \le \mu, \mu' \le r).$$

Let $B \in \mathbb{K}^{I \times I}$ be the corresponding matrix, where $I = \{1, \ldots, r_j\} \times \{1, \ldots, r\}$. The orthonormality of $\{\mathbf{b}_{\nu}^{(j)}\}$ is equivalent to $\sum_{\ell} B_{(\nu,\ell),(\nu',\ell)} = \delta_{\nu,\nu'}$. Note that $B = B^{\mathrm{H}}$.

Consider the tensor $\mathbf{v} = \sum_{\nu=1}^{r_j} \sum_{\mu=1}^r c_{\nu\mu} \mathbf{b}_{\nu}^{(j)} \otimes u_{\mu}$. The normalisation $\|\mathbf{v}\| = 1$ gives $\sum_{\nu,\mu} |c_{\nu\mu}|^2 = 1$. The entries $c_{\nu\mu}$ define the vector $c \in \mathbb{K}^I$.

Theorem 5.10 The spectrum of B is bounded by 1. The above defined tensor \mathbf{v} is symmetric if and only if c is an eigenvector of B corresponding to the eigenvalue 1.

Proof. Let $\mathbf{s} = S_{j+1}\mathbf{v}$. The projection property of S_{j+1} implies that $\langle \mathbf{v}, \mathbf{s} \rangle \leq 1$. Criterion 5.9 states that \mathbf{v} is symmetric (i.e., $\mathbf{v} = \mathbf{s}$) if and only if $\langle \mathbf{v}, \mathbf{s} \rangle = 1$. Calculating the scalar product according to §5.4.3 yields $(j+1) \langle \mathbf{v}, \mathbf{s} \rangle = 1 + j (Bc, c)$, where (\cdot, \cdot) is the Euclidean product of \mathbb{K}^I . The inequality $\langle \mathbf{v}, \mathbf{s} \rangle \leq 1$ shows that all eigenvalues of B are bounded by 1. The equality $\langle \mathbf{v}, \mathbf{s} \rangle = 1$ requires that $(Bc, c) = 1 = \max\{(Bc', c') : \|c'\| = 1\}$, i.e., c is the eigenvector with eigenvalue $\lambda = 1$.

The questions from above take now the following form: (a) How can we ensure that 1 belongs to the spectrum of B, (b) what is the dimension of the corresponding eigenspace?

5.4.5 Examples

The following examples use tensors of order d = 3. The case d = 2 is too easy since tensors of $\otimes^2 U$ correspond to matrices via $\mathbf{v} = \sum_{\nu,\mu=1}^r c_{\nu\mu} u_{\nu} \otimes u_{\mu} \mapsto C := (c_{\nu\mu})_{\nu,\mu=1}^r$. Hence symmetric tensors \mathbf{v} are characterised by symmetric matrices C.

In the following examples $u_1 = a, u_2 = b \in V$ are orthonormal vectors. A possible choice is $V = \mathbb{K}^2$.

Example 5.11 We want to represent the symmetric tensor $\mathbf{s} := a \otimes a \otimes a$. We use $U = \operatorname{span}\{a, b\}$ and the symmetric subspace $\mathbf{U}_2 := \operatorname{span}\{\mathbf{b}_1^{(2)}\} \subset \mathcal{S}(U \otimes U) \subset U \otimes U$ with $\mathbf{b}_1^{(2)} := a \otimes a$. Symmetrisation of $\mathbf{U}_2 \otimes U = \operatorname{span}\{a \otimes a \otimes a, a \otimes a \otimes b\}$ yields $\mathcal{S}(\mathbf{U}_2 \otimes U) = \operatorname{span}\{a \otimes a \otimes a, \frac{1}{3}(a \otimes a \otimes b + a \otimes b \otimes a + b \otimes a \otimes a)\}$. Obviously, $\mathcal{S}(\mathbf{U}_2 \otimes U)$ is not a subspace of $\mathbf{U}_2 \otimes U$.

The reason for $\mathcal{S}(\mathbf{U}_2 \otimes U) \not\subset \mathbf{U}_2 \otimes U$ in Example 5.11 may be seen in the choice of $U = \operatorname{span}\{a, b\}$. This space is larger than necessary: $U = U_1^{\min}(\mathbf{s}) = \operatorname{span}\{a\}$ is sufficient and this choice leads to $\mathcal{S}(\mathbf{U}_2 \otimes U) = \mathbf{U}_2 \otimes U$.

In the next example, U is chosen as $U_1^{\min}(\mathbf{s})$.

Example 5.12 We want to represent the symmetric tensor $\mathbf{s} := a \otimes a \otimes a + b \otimes b \otimes b$. We use $U = \operatorname{span}\{a, b\}$ and the symmetric subspace $\mathbf{U}_2 := \operatorname{span}\{\mathbf{b}_1^{(2)}, \mathbf{b}_2^{(2)}\} \subset \mathcal{S}(U \otimes U) \subset U \otimes U$ with $\mathbf{b}_1^{(2)} := a \otimes a$ and $\mathbf{b}_2^{(2)} := b \otimes b$. The tensor space $\mathbf{U}_2 \otimes U$ is spanned by $a \otimes a \otimes a$, $b \otimes b \otimes b$, $a \otimes a \otimes b$, $b \otimes b \otimes a$. The first two tensors are already symmetric. The symmetrisation of $a \otimes a \otimes b$ leads to a tensor which is not contained in $\mathbf{U}_2 \otimes U$. The same holds for the last tensor. Hence, $\mathcal{S}(\mathbf{U}_2 \otimes U) \not\subset \mathbf{U}_2 \otimes U$.

In Examples 5.11 and 5.12, we can omit the tensors $\mathbf{b}_i^{(2)} \otimes u_j$ whose symmetrisation does not belong to $\mathbf{U}_2 \otimes U$, and still obtain a subspace containing the tensor **s** to be represented. The latter statement is not true in the third example.

Example 5.13 We want to represent the symmetric tensor $\mathbf{s} := \otimes^3 (a+b) + \otimes^3 (a-b)$. We use $U = \operatorname{span}\{a,b\}$ and the symmetric subspace $\mathbf{U}_2 := \operatorname{span}\{\mathbf{b}_1^{(2)}, \mathbf{b}_2^{(2)}\} \subset \mathcal{S}(U \otimes U) \subset U \otimes U$ with $\mathbf{b}_1^{(2)} := \otimes^2 (a+b)$ and $\mathbf{b}_2^{(2)} := \otimes^2 (a-b)$. The tensor space $\mathbf{U}_2 \otimes U$ is spanned by four tensors $\mathbf{b}_i^{(2)} \otimes u_j$. For i = j = 1, we have $\mathbf{b}_1^{(2)} \otimes a = (a+b) \otimes (a+b) \otimes a$, whose symmetrisation does not belong to $\mathbf{U}_2 \otimes U$. The same holds for the other three tensors. Hence, $\mathcal{S}(\mathbf{U}_2 \otimes U) \not\subset \mathbf{U}_2 \otimes U$.

Note that the setting of Example 5.13 coincides with Example 5.12 when we replace the orthonormal basis $\{u_1 = a, u_2 = b\}$ with $\{u_1 = (a+b)/\sqrt{2}, u_2 = (a-b)/\sqrt{2}\}$.

The next example underlines the important role of condition $\mathbf{U}_{j}^{\min}(\mathbf{v}) \subset \mathbf{U}_{j}$.

Example 5.14 Let $\mathbf{U}_2 := \operatorname{span}\{\mathbf{b}_1^{(2)}\}$ with $\mathbf{b}_1^{(2)} := a \otimes b + b \otimes a$. A general tensor in $\mathbf{U}_2 \otimes U$ has the form $\mathbf{b}_1^{(2)} \otimes (\alpha a + \beta b)$. There is no symmetric tensor of this form, except the zero tensor $(\alpha + \beta = 0)$. This shows that \mathbf{U}_2 is too small: there is no nontrivial symmetric tensor \mathbf{v} with $\mathbf{U}_2^{\min}(\mathbf{v}) \subset \mathbf{U}_2$.

5.4.6 Open Questions About $S(\mathbf{U}_j \otimes U) \cap (\mathbf{U}_j \otimes U)$

We repeat the definition $\hat{\mathbf{U}}_{j+1} := \mathcal{S}(\mathbf{U}_j \otimes U) \cap (\mathbf{U}_j \otimes U)$. The main questions are:

- What is the dimension of $\hat{\mathbf{U}}_{j+1}$, in particular, compared with $\dim(\mathbf{U}_j^{\min}(\mathbf{v}))$, if \mathbf{v} is the tensor to be represented?
- Is there a constructive description of $\hat{\mathbf{U}}_{i+1}$?

The minimal set, which is needed for the construction of the tensors in $\hat{\mathbf{U}}_{i+1}$, is

$$\check{\mathbf{U}}_j := \sum_{\mathbf{v} \in \hat{\mathbf{U}}_{j+1}} \mathbf{U}_j^{\min}(\mathbf{v}).$$

By definition, $\check{\mathbf{U}}_j \subset \mathbf{U}_j$ holds, but it is not obvious whether $\check{\mathbf{U}}_j = \hat{\mathbf{U}}_j$. This yields the next question:

• Does $\check{\mathbf{U}}_i = \mathbf{U}_i$ hold?

In the negative case, there is a direct sum $\mathbf{U}_j = \check{\mathbf{U}}_j \oplus \mathbf{Z}_j$, where $\mathbf{Z}_j \neq \{0\}$ contains symmetric tensors in $\mathbf{V}_{sym}^{(j)}$ which cannot be continued to symmetric tensors in $\mathbf{V}_{sym}^{(j+1)}$. Using \mathbf{U}_j instead of $\check{\mathbf{U}}_j$ would be inefficient.

5.4.7 Answers for d = 3 and r = 2

The questions from above can be answered for the simple case of d = 3 (transfer from d = 2 to d = 3) and r = 2. Hence we have

$$\dim(U) = 2, \quad \mathbf{U}_1 = U, \quad \mathbf{U}_2 \subset \mathbf{U}_{\mathrm{sym}}^{(2)}$$

and have to investigate the space $\hat{\mathbf{U}}_3 := \mathcal{S}_3(\mathbf{U}_2 \otimes U) \cap (\mathbf{U}_2 \otimes U)$. We recall that $\check{\mathbf{U}}_2 = \sum_{\mathbf{w} \in \hat{\mathbf{U}}_3} \mathbf{U}_2^{\min}(\mathbf{w}) \subset \mathbf{U}_2$ is the smallest subspace of \mathbf{U}_2 with the property $\mathcal{S}_3(\check{\mathbf{U}}_2 \otimes U) \cap (\check{\mathbf{U}}_2 \otimes U) = \hat{\mathbf{U}}_3$. Hence, if $\dim(\mathbf{U}_2) > \dim(\check{\mathbf{U}}_2)$, \mathbf{U}_2 contains tensor which are useless for the construction of symmetric tensor in $\hat{\mathbf{U}}_3$.

The symmetric tensors $\mathbf{v} \in \mathbf{U}_2$ correspond to symmetric 2×2 matrices. Since $\dim(\mathbf{U}_{sym}^{(2)}) = 3$, the following list of cases is complete. The general assumption of the following theorems is $\dim(U) = 2$.

Theorem 5.15 (Case dim $(\mathbf{U}_2) = 1$) Let dim $(\mathbf{U}_2) = 1$ and $\mathbf{U}_2 = \operatorname{span}\{\mathbf{b}_1\} \subset \mathbf{U}_{\operatorname{sym}}^{(2)}$. If rank $(\mathbf{b}_1) = 1$ then

$$\mathbf{\check{U}}_2 = \mathbf{U}_2, \quad \dim(\mathbf{\hat{U}}_3) = 1;$$

otherwise we have $\operatorname{rank}(\mathbf{b}_1) = 2$ and

$$\mathbf{\check{U}}_2 = \{0\} \subset \mathbf{U}_2, \quad \mathbf{\hat{U}}_3 = \{0\}$$

Proof. Note that $\operatorname{rank}(\mathbf{b}_1) \leq \dim(U) = 2$. $\operatorname{rank}(\mathbf{b}_1) = 0$ is excluded because of $\mathbf{b}_1 = 0$ and the assumption that $\mathbf{U}_2 = \operatorname{span}\{\mathbf{b}_1\}$ is one-dimensional. Hence, $\operatorname{rank}(\mathbf{b}_1)$ only takes the values 1 and 2.

If rank $(\mathbf{b}_1) = 1$, $\mathbf{b}_1 = a \otimes a'$ follows. Symmetry shows that $\mathbf{b}_1 = a \otimes a$ (possibly after changing the sign⁵). Then

$$\mathbf{\hat{U}}_3 = \operatorname{span}\{\mathbf{b}_1 \otimes a\} = \operatorname{span}\{a \otimes a \otimes a\}.$$

If rank(\mathbf{b}_1) = 2, the general form of $\mathbf{w} \in \mathbf{U}_2 \otimes U$ is $\mathbf{w} = \mathbf{b}_1 \otimes (\xi a + \eta b)$. Assume $(\xi, \eta) \neq 0$. Then the only symmetric tensor of this form is $\mathbf{w} = \otimes^3(\xi a + \eta b)$, i.e., $\mathbf{b}_1 = (\xi a + \eta b) \otimes (\xi a + \eta b)$. The contradiction follows from rank(\mathbf{b}_1) = 1. Hence $\xi = \eta = 0$ leads to the assertion.

The statements about $\check{\mathbf{U}}_2$ follow from the definition $\check{\mathbf{U}}_2 = \mathbf{U}_2^{\min}(\hat{\mathbf{U}}_3)$.

Theorem 5.16 (dim $(U_2) = 2$) Let dim $(U_2) = 2$. Then

$$\mathbf{\check{U}}_2 = \mathbf{U}_2, \quad \dim(\mathbf{\hat{U}}_3) = 2.$$

The precise characterisation of $\hat{\mathbf{U}}_3 \subset \mathbf{U}_{sym}^{(3)}$ is given in the proof.

Proof. (i) There are two linearly independent and symmetric tensors \mathbf{b}_1 , \mathbf{b}_2 with $\mathbf{U}_2 = \operatorname{span}\{\mathbf{b}_1, \mathbf{b}_2\}$. Fixing linearly independent vectors $a, b \in U = \operatorname{span}\{a, b\}$, the tensors have the form

$$\mathbf{b}_1 = \alpha \, a \otimes a + \beta \, b \otimes b + \gamma \, (a \otimes b + b \otimes a) \,, \\ \mathbf{b}_2 = \alpha' a \otimes a + \beta' b \otimes b + \gamma' \, (a \otimes b + b \otimes a)$$

In part (vi) we shall prove that $\dim(\hat{\mathbf{U}}_3) \leq 2$. The discussion of the cases 1–3 will show that $\dim(\hat{\mathbf{U}}_3) \geq 2$, so that $\dim(\hat{\mathbf{U}}_3) = 2$ follows.

(ii) Case 1: $\gamma = \gamma' = 0$. One concludes that $\mathbf{U}_2 = \operatorname{span}\{a \otimes a, b \otimes b\}$. Then the first case in Theorem 5.15 shows that $a \otimes a \otimes a$ and $b \otimes b \otimes b$ belong to $\hat{\mathbf{U}}_3$ so that $\dim(\hat{\mathbf{U}}_3) \geq 2$ and part (vi) prove

$$\hat{\mathbf{U}}_3 = \operatorname{span}\{a \otimes a \otimes a, b \otimes b \otimes b\}.$$
(5.12)

(iii) Case 2: $(\gamma, \gamma') \neq 0$. W.l.o.g. assume $\gamma \neq 0$. We introduce the matrices

$$M_{\alpha} := \begin{bmatrix} \alpha & \alpha' \\ \gamma & \gamma' \end{bmatrix}, \qquad M_{\beta} := \begin{bmatrix} \gamma & \gamma' \\ \beta & \beta' \end{bmatrix}.$$

Since $\gamma \neq 0$, both matrices have a rank ≥ 1 . If rank $(M_{\alpha}) = \operatorname{rank}(M_{\beta}) = 1$, (α, β, γ) and $(\alpha', \beta', \gamma')$ would be linearly dependent in contradiction to the linear independence of $\{\mathbf{b}_1, \mathbf{b}_2\}$. Hence, at least one matrix has rank 2 and is regular. W.l.o.g. we assume that rank $(M_{\alpha}) = 2$ (otherwise interchange the roles of a and b).

(iv) For any $(A, B) \in \mathbb{K}^2$ the system

$$M_{\alpha} \begin{bmatrix} \xi \\ \eta \end{bmatrix} = M_{\beta} \begin{bmatrix} A \\ B \end{bmatrix}$$
(5.13)

can be solved for $(\xi, \eta) \in \mathbb{K}^2$. Then the tensor

$$\mathbf{w} := (A\mathbf{b}_1 + B\mathbf{b}_2) \otimes a + (\xi\mathbf{b}_1 + \eta\mathbf{b}_2) \otimes b$$

⁵ If $\mathbb{K} = \mathbb{C}$, the representation $\mathbf{b}_1 = a \otimes a$ holds in the strict sense, If $\mathbb{K} = \mathbb{R}$, either $\mathbf{b}_1 = a \otimes a$ or $\mathbf{b}_1 = -a \otimes a$ can be obtained. Since the purpose of \mathbf{b}_1 is to span the subspace, we may w.l.o.g. replace $\mathbf{b}_1 = -a \otimes a$ by $\mathbf{b}_1 = a \otimes a$.

is symmetric and belongs to $\hat{\mathbf{U}}_3$. For a proof apply Lemma 5.3: $\mathbf{w} \in \mathbf{U}_{sym}^{(3)}$ is equivalent to $\varphi_b (A\mathbf{b}_1 + B\mathbf{b}_2) = \varphi_a (\xi \mathbf{b}_1 + \eta \mathbf{b}_2)$, where the functionals defined by $\varphi_a(a) = \varphi_b(b) = 1$, $\varphi_a(b) = \varphi_b(a) = 0$ apply to the last argument. The latter equation is equivalent to (5.13).

Let (ξ, η) be the solution of (5.13) for (A, B) = (1, 0), while (ξ', η') is the solution for (A, B) = (0, 1). Hence we have found a two-dimensional subspace

$$\operatorname{span}\{\mathbf{b}_1 \otimes a + (\xi \mathbf{b}_1 + \eta \mathbf{b}_2) \otimes b, \ \mathbf{b}_2 \otimes a + (\xi' \mathbf{b}_1 + \eta' \mathbf{b}_2) \otimes b\} \subset \hat{\mathbf{U}}_3.$$
(5.14)

(v) In both cases (5.12) and (5.14) the minimal subspace $\check{\mathbf{U}}_2 = \mathbf{U}_2^{\min}(\hat{\mathbf{U}}_3)$ coincides with \mathbf{U}_2 .

(vi) For an indirect proof of dim $(\hat{\mathbf{U}}_3) \leq 2$ assume dim $(\hat{\mathbf{U}}_3) \geq 3$. Let $\varphi_a : \hat{\mathbf{U}}_3 \to \mathbf{U}_2^{\min}(\hat{\mathbf{U}}_3) = \mathbf{U}_2$ be the mapping $\mathbf{w} = \mathbf{v}_1 \otimes a + \mathbf{v}_2 \otimes b \mapsto \mathbf{v}_1$. Since dim $(\hat{\mathbf{U}}_3) > \dim(\mathbf{U}_2)$, there is some $\mathbf{w} \in \hat{\mathbf{U}}_3, \mathbf{w} \neq 0$ with $\varphi_a(\mathbf{w}) = 0$. This implies $\mathbf{w} = \mathbf{v}_2 \otimes b$ and therefore, by symmetry, $\mathbf{w} = b \otimes b \otimes b$ up to a nonzero factor. Similarly, there are an analogously defined functional φ_b and $\mathbf{w} \in \hat{\mathbf{U}}_3, \mathbf{w} \neq 0$ with $\varphi_b(\mathbf{w}) = 0$ proving $a \otimes a \otimes a \in \hat{\mathbf{U}}_3$. From $a \otimes a \otimes a, b \otimes b \otimes b \in \hat{\mathbf{U}}_3$ we conclude that $\check{\mathbf{U}}_2 := \mathbf{U}_2^{\min}(\hat{\mathbf{U}}_3) \supset \operatorname{span}\{a \otimes a, b \otimes b\}$. Then $\check{\mathbf{U}}_2 \subset \mathbf{U}_2$ and dim $(\mathbf{U}_2) = 2$ prove dim $(\hat{\mathbf{U}}_3) \leq 2$.

Theorem 5.17 (dim(\mathbf{U}_2) = 3) If dim(\mathbf{U}_2) = 3, \mathbf{U}_2 coincides with space $\mathbf{U}_{sym}^{(2)}$ of all symmetric tensors in $U \otimes U$ and generates all tensors in $\mathbf{U}_{sym}^{(3)}$:

$$\mathbf{\check{U}}_2 = \mathbf{U}_2 = \mathbf{U}_{sym}^{(2)}, \quad \mathbf{\hat{U}}_3 = \mathbf{U}_{sym}^{(3)} \quad with \quad \dim(\mathbf{\hat{U}}_3) = 4.$$

Proof. The statements follow from $\dim(\mathbf{U}_{sym}^{(2)}) = 3$.

5.5 Direct Use of $U_i^{\min}(\mathbf{v})$

Statement (5.4) emphasises the important role of the minimal subspace $\mathbf{U}_{i}^{\min}(\mathbf{v})$.

5.5.1 Case of Known $U_i^{\min}(\mathbf{v})$

If the minimal subspaces $\mathbf{U}_{j}^{\min}(\mathbf{v})$ of a symmetric tensor $\mathbf{v} \in \mathbf{U}_{\text{sym}}^{(d)}$ are given, the above problems disappear. In this case we may define $\mathbf{U}_{j} := \mathbf{U}_{j}^{\min}(\mathbf{v})$. This ensures that

$$\check{\mathbf{U}}_j = \mathbf{U}_j \quad \text{and} \quad \hat{\mathbf{U}}_{j+1} \supset \mathbf{U}_{j+1}^{\min}(\mathbf{v})$$

(cf. Theorem 5.4).

If we want to be able to represent all tensors of a subspace $\mathbf{V}_0 = \operatorname{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_k\} \subset \mathbf{U}_{\operatorname{sym}}^{(d)}$, we may use

$$\mathbf{U}_j := \mathbf{U}_j^{\min}(\mathbf{V}_0) = \sum_{
u=1}^k \mathbf{U}_j^{\min}(\mathbf{v}_
u)$$

Lemma 6.1 shows that \mathbf{U}_j satisfies (6.2).

Next we consider the case that $\mathbf{U}_{i}^{\min}(\mathbf{v})$ is not given explicitly, but can be determined by symmetrisation.

5.5.2 Case of $\mathbf{v} = \mathcal{S}(\mathbf{w})$

As in §2.1 we assume that the symmetric tensor $0 \neq \mathbf{v} \in \mathbf{U}_{sym}^{(d)}$ is the symmetrisation $\mathcal{S}(\mathbf{w})$ of a known tensor $\mathbf{w} \in \otimes^d V$. Unlike in §2.1, we assume that \mathbf{w} is given in the TT format with minimal subspaces⁶ $\mathbf{U}_j^{\min}(\mathbf{w})$. The obvious task is to transfer $\mathbf{U}_j^{\min}(\mathbf{w})$ into $\mathbf{U}_j^{\min}(\mathbf{v}) = \mathbf{U}_j^{\min}(\mathcal{S}(\mathbf{w}))$.

We solve this problem by induction on $d = 1, \ldots$. The proof also defines an recursive algorithm.

For d = 1 nothing is to be done since $\mathbf{v} = \mathcal{S}(\mathbf{w}) = \mathbf{w}$. Formally, $\mathbf{U}_0^{\min}(\mathbf{v})$ is the field \mathbb{K} and $U_1 \subset \mathbb{K} \otimes U$ corresponds to (4.3).

The essential part of the proof and of the algorithm is the step from d-1 to d.

 $^{^{6}}$ In the case of hierarchical tensor representations it is easy to reduce the subspaces to the minimal ones by introducing the HOSVD bases (cf. Hackbusch [9, §11.3.3]).

Lemma 5.18 Let $S_{[j]} : \otimes^d V \to \otimes^d V$ $(1 \le j \le d)$ be the symmetrisation operator S_{d-1} in (1.8) applied to the directions $D \setminus \{j\}$ (cf. (1.2)). Using the transpositions π_{1j}, π_{j1} , the explicit definition is

$$\mathcal{S}_{[j]} = \pi_{1j} \ (id \otimes \mathcal{S}_{d-1}) \ \pi_{j1}$$

Then the symmetrisation operator S_d is equal to

$$\mathcal{S}_d = rac{1}{d} \sum_{j=1}^d \mathcal{S}_{[j]} \pi_{dj}$$

This lemma proves the next result.

Conclusion 5.19 Let $\mathbf{w} \in \otimes^d U$ and $\varphi \in U'$. Then

$$\varphi^{(d)}(\mathcal{S}_d \mathbf{w}) = \frac{1}{d} \mathcal{S}_{d-1} \sum_{j=1}^d \varphi^{(j)}(\mathbf{w})$$

holds with $\varphi^{(j)}$ defined in (1.6).

The $\{1, \ldots, d-1\}$ -plex rank r_{d-1} of $\mathbf{x} \in \otimes^d U$ introduced by Hitchcock [11] is the smallest r_{d-1} with $\mathbf{x} = \sum_{\nu=1}^{r_{d-1}} \mathbf{x}_{\nu} \otimes y_{\nu}$ ($\mathbf{x}_{\nu} \in \otimes^{d-1} U, y_{\nu} \in U$). For instance, this representation is the result of the HOSVD representation (cf. [9, §11.3.3]). The minimal subspace $\mathbf{U}_{d-1}^{\min}(\mathbf{x})$ is the span of $\{\mathbf{x}_{\nu} : 1 \leq \nu \leq r_{d-1}\}$.

Alternatively, choose the standard basis $\{u_{\nu} : 1 \leq \nu \leq r\}$ of U and the representation $\mathbf{x} = \sum_{\nu=1}^{r} \mathbf{z}_{\nu} \otimes u_{\nu}$ together with the dual basis $\{\varphi_{\nu}\}$ of $\{u_{\nu}\}$. Then the tensors $\mathbf{z}_{\nu} = \varphi_{\nu}(\mathbf{x})$ may be linearly dependent so that some of them may be omitted. Let \mathbf{x}_{ν} $(1 \leq \nu \leq r_{d-1})$ be the remaining ones: $\mathbf{U}_{d-1}^{\min}(\mathbf{x}) = \operatorname{span}\{\mathbf{x}_{\nu} : 1 \leq \nu \leq r_{d-1}\}$.

Remark 1.5 states that

$$\mathbf{U}_{d-2}^{\min}(\mathbf{x}) = \mathbf{U}_{d-2}^{\min}(\mathbf{U}_{d-1}^{\min}(\mathbf{x})) = \sum_{\nu=1}^{r_{d-1}} \mathbf{U}_{d-2}^{\min}(\mathbf{x}_{\nu}).$$
(5.15)

This allows us to determine the minimal subspaces recursively.

Let the TT representation of $\mathbf{w} \in \otimes^d U$ be given. The TT format is also called the matrix product representation since $\mathbf{w} \in \otimes^d U$ can be written as

$$\mathbf{w} = \sum_{k_1, k_2, \dots, k_{d-1}} v_{1, k_1}^{(1)} \otimes v_{k_1, k_2}^{(2)} \otimes v_{k_2, k_3}^{(3)} \otimes \dots \otimes v_{k_{d-1}, 1}^{(d)},$$

where the vectors $v_{k_j,k_{j+1}}^{(j)} \in U$ are data available from the TT representation. k_j varies in an index set I_j with $\#I_j = \dim(\mathbf{U}_j^{\min}(\mathbf{w}))$. The tensor $\varphi^{(j)}(\mathbf{w}) \in \otimes^{d-1}U$ takes the matrix product form

$$\varphi^{(j)}(\mathbf{w}) = \sum_{k_{j-1}, k_j} \varphi(v_{k_{j-1}, k_j}^{(j)}) \sum_{\substack{k_1, \dots, k_{j-2}, \\ k_{j+1}, \dots, k_{d-1}}} v_{1, k_1}^{(1)} \otimes \dots \otimes v_{k_{j-2}, k_{j-1}}^{(j-1)} \otimes v_{k_j, k_{j+1}}^{(j+1)} \otimes \dots \otimes v_{k_{d-1}, 1}^{(d)}$$

These tensors can be added within the TT format: $\mathbf{w}_{\nu} := \sum_{j=1}^{d} \varphi_{\nu}^{(j)}(\mathbf{w}) \in \otimes^{d-1} U$. We conclude that

$$\mathbf{U}_{d-1}^{\min}(\mathbf{v}) = \mathbf{U}_{d-1}^{\min}(\mathcal{S}_d \mathbf{w}) = \operatorname{span}\{\mathcal{S}_{d-1}\mathbf{w}_{\nu} : 1 \le \nu \le r_{d-1}\}.$$

According to (5.15) the next minimal subspace $\mathbf{U}_{d-2}^{\min}(\mathbf{v})$ can be written as $\sum_{\nu} \mathbf{U}_{d-2}^{\min}(\mathcal{S}_{d-1}\mathbf{w}_{\nu})$ so that we can apply the inductive hypothesis.

6 Operations

The computation of scalar products is already discussed. Next we investigate the tensor addition.

Assume that \mathbf{v}' and \mathbf{v}'' are two symmetric tensors represented by subspaces \mathbf{U}'_k and \mathbf{U}''_k and corresponding bases. For k = 1, we use the notation $U' := \mathbf{U}'_1$ and $U'' := \mathbf{U}''_1$. By assumption, we have

$$\mathbf{U}_{k+1}^{\min}(\mathbf{v}') \subset \mathbf{U}_{k+1}' \subset \mathcal{S}_{k+1}(\mathbf{U}_k' \otimes U') \cap (\mathbf{U}_k' \otimes U'), \qquad (6.1a)$$

$$\mathbf{U}_{k+1}^{\min}(\mathbf{v}'') \subset \mathbf{U}_{k+1}'' \subset \mathcal{S}_{k+1}(\mathbf{U}_k'' \otimes U'') \cap (\mathbf{U}_k'' \otimes U'').$$
(6.1b)

Lemma 6.1 The sum $\mathbf{s} := \mathbf{v}' + \mathbf{v}''$ can be represented by the subspaces

$$\mathbf{U}_k := \mathbf{U}'_k + \mathbf{U}''_k, \qquad U := U' + U''.$$

These spaces satisfy again the conditions

$$\mathbf{U}_{k+1}^{\min}(\mathbf{s}) \subset \mathbf{U}_{k+1} \subset \mathcal{S}_{k+1}(\mathbf{U}_k \otimes U) \cap (\mathbf{U}_k \otimes U).$$
(6.2)

Proof. The inclusions (6.1a,b) imply

$$\mathbf{U}_{k+1}^{\min}(\mathbf{v}') + \mathbf{U}_{k+1}^{\min}(\mathbf{v}'') \subset \mathbf{U}_{k+1} = \mathbf{U}_{k+1}' + \mathbf{U}_{k+1}''$$

$$\subset (\mathcal{S}_{k+1}(\mathbf{U}_k' \otimes U') \cap (\mathbf{U}_k' \otimes U')) + (\mathcal{S}_{k+1}(\mathbf{U}_k'' \otimes U'') \cap (\mathbf{U}_k'' \otimes U'')).$$

Since $\mathbf{U}_{k+1}^{\min}(\mathbf{s}) \subset \mathbf{U}_{k+1}^{\min}(\mathbf{v}') + \mathbf{U}_{k+1}^{\min}(\mathbf{v}'')$, the first part of (6.2) follows: $\mathbf{U}_{k+1}^{\min}(\mathbf{s}) \subset \mathbf{U}_{k+1}$. The inclusion $\mathbf{U}_{k}' \otimes U' \subset \mathbf{U}_{k} \otimes U$ implies that

$$\mathcal{S}_{k+1}(\mathbf{U}_k' \otimes U') \cap (\mathbf{U}_k' \otimes U') \subset \mathcal{S}_{k+1}(\mathbf{U}_k \otimes U) \cap (\mathbf{U}_k \otimes U)$$

The analogous statement for $\mathcal{S}_{k+1}(\mathbf{U}_k'' \otimes U'') \cap (\mathbf{U}_k'' \otimes U'')$ yields

$$(\mathcal{S}_{k+1}(\mathbf{U}'_k \otimes U') \cap (\mathbf{U}'_k \otimes U')) + (\mathcal{S}_{k+1}(\mathbf{U}''_k \otimes U'') \cap (\mathbf{U}''_k \otimes U'')) \\ \subset \mathcal{S}_{k+1}(\mathbf{U}_k \otimes U) \cap (\mathbf{U}_k \otimes U).$$

Hence also the second part of (6.2) is proved.

The computation of the orthonormal basis of \mathbf{U}_k is performed in the order k = 1, 2, ... As soon as orthonormal bases of \mathbf{U}_k and U are given, the orthonormal basis of \mathbf{U}_{k+1} can be determined.

Since the spaces $\mathbf{U}_k = \mathbf{U}'_k + \mathbf{U}''_k$ may be larger than necessary, a truncation is advisable.

7 Truncation

The standard truncation procedure uses the SVD. Formally, we have for any tensor $\mathbf{u} \in \mathbf{V}$ and any $k \in \{1, \ldots, d-1\}$ a singular value decomposition

$$\mathbf{u} = \sum_{\nu=1}^{r_u} \sigma_\nu \mathbf{v}_\nu \otimes \mathbf{w}_\nu, \tag{7.1}$$

where $\{\mathbf{v}_{\nu} : 1 \leq \nu \leq r_u\} \subset \otimes^k V$ and $\{\mathbf{w}_{\nu} : 1 \leq \nu \leq r_u\} \subset \otimes^{d-k} V$ are orthonormal systems and $\{\sigma_1 \geq \sigma_2 \geq \ldots\}$ are the singular values. The usual approach is to choose some $s < r_u$ and to define the tensor

$$\hat{\mathbf{u}} = \sum_{\nu=1}^{s} \sigma_{\nu} \mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$$

which can be represented with subspaces of lower dimension.

In the case of symmetric tensors $\mathbf{u} \in \mathbf{V}_{sym}^{(d)}$, we have $\mathbf{v}_{\nu} \in \mathbf{V}_{sym}^{(k)}$ and $\mathbf{w}_{\nu} \in \mathbf{V}_{sym}^{(d-k)}$. However, the standard truncation cannot be used since there is no guarantee that the truncated tensor $\hat{\mathbf{u}} = \sum_{\nu=1}^{s} \sigma_{\nu} \mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$ again belongs to $\mathbf{V}_{sym}^{(d)}$.

7.1 Truncation for k = 1 and k = d - 1

In the cases k = 1 and k = d - 1, the truncation can be performed as follows. For k = 1, the standard truncation $\mathbf{u} \mapsto \hat{\mathbf{u}}$ can be written as $\hat{\mathbf{u}} = (P \otimes \mathbf{I}) \mathbf{u}$, where $P : V \to V$ is the orthogonal projection onto the subspace

$$\tilde{U} := \operatorname{span}\{\mathbf{v}_{\nu} : 1 \le \nu \le s\} \subset V$$

while $\mathbf{I} = \otimes^{d-1} I$ is the identity on $\otimes^{d-1} V$.

In the symmetric case, we need a symmetric mapping. If we delete the components $\{\mathbf{v}_{\nu} : \nu > s\}$ in the first direction, the same must be done in the other directions. The corresponding mapping is the orthogonal projection

$$\mathbf{P} := \otimes^d P$$

onto the subspace $\hat{\mathbf{U}}_{sym}^{(d)} \subset \mathbf{V}_{sym}^{(d)}$. Note that the error $\mathbf{u} - \mathbf{P}\mathbf{u}$ does not only consist of the omitted terms $\sum_{\nu=s+1}^{r_u} \sigma_{\nu} \mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$, but also of $\sum_{\nu=1}^{s} \sigma_{\nu} \mathbf{v}_{\nu} \otimes (\mathbf{I} - \otimes^{d-1}P) \mathbf{w}_{\nu}$.

In the case of k = d - 1, \mathbf{w}_{ν} belongs to V and the analogous construction can be performed. If d = 3, the cases k = 1 and k = d - 1 cover all possible ones.

7.2 Open Problem for 1 < k < d - 1

If d > 3, there are integers k with 1 < k < d - 1. Then both \mathbf{v}_{ν} and \mathbf{w}_{ν} in (7.1) are tensors of order ≥ 2 . It is not obvious how the analogue of the previous mapping \mathbf{P} could look like. The advantage of a symmetric projection \mathbf{P} would be the existence of a tensor $\mathbf{v}' = \mathbf{P}\mathbf{v} \in \mathbf{U}_{sym}$. Define $\mathbf{w}' := \sum_{\nu=1}^{s} \sigma_{\nu}\mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$ and $\mathbf{w}'' := \sum_{\nu=s+1}^{r_{u}} \sigma_{\nu}\mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$ by SVD. Assume that $\mathbf{P}\mathbf{w}' \neq 0$ while $\mathbf{P}\mathbf{w}'' = 0$. Then

$$\mathbf{P}\mathbf{v} = \mathbf{P}\mathcal{S}(\mathbf{w}' + \mathbf{w}'') = \mathcal{S}(\mathbf{P}\mathbf{w}' + \mathbf{P}\mathbf{w}'') = \mathcal{S}(\mathbf{P}\mathbf{w}')$$

(cf. Lemma 9.1) does not vanish, i.e., $\mathbf{v}' \neq 0$ ensures the existence of a nontrivial subspaces $\mathbf{U}_j^{\min}(\mathbf{v}')$ $(1 \leq j \leq d)$.

Let $P_k : \mathbf{V}_{sym}^{(k)} \to \mathbf{V}_{sym}^{(k)}$ be the orthogonal projection onto $\operatorname{span}\{\mathbf{v}_{\nu} : 1 \leq \nu \leq s\}$, so that $\mathbf{P}_k := P_k \otimes (\otimes^{d-k}I)$ maps \mathbf{u} to the SVD truncation $\hat{\mathbf{u}} = \sum_{\nu=1}^s \sigma_{\nu} \mathbf{v}_{\nu} \otimes \mathbf{w}_{\nu}$. The symmetrisation $\mathbf{P} = \mathcal{S}(\mathbf{P}_k)$ defines $\mathbf{u}' := \mathbf{Pu} \in \mathbf{U}_{sym}^{(d)}$. Since

$$\langle \mathbf{u}, \mathbf{u}'
angle = \langle \mathbf{u}, \mathbf{P}\mathbf{u}
angle = \langle \mathbf{u}, \mathcal{S}(\mathbf{P}_k)\mathbf{u}
angle = \langle \mathbf{u}, \mathcal{S}(\mathbf{P}_k\mathbf{u})
angle = \langle \mathcal{S}(\mathbf{u}), \mathbf{P}_k\mathbf{u}
angle = \langle \mathbf{u}, \mathbf{P}_k\mathbf{u}
angle = \langle \mathbf{\hat{u}}, \mathbf{\hat{u}}
angle,$$

the tensor \mathbf{u}' does not vanish. However, it is not obvious that $\dim(\mathbf{U}_k^{\min}(\mathbf{u}')) \leq s$ holds, as intended by the truncation.

A remedy is a follows. Assume that the (not truncated) tensor uses the subspaces \mathbf{U}_j satisfying (5.2). Let the SVD for index k reduce \mathbf{U}_k to \mathbf{U}'_k . Since $\mathbf{U}'_k \subset \mathbf{U}_k$, \mathbf{U}'_k still belongs to $\mathbf{U}^{(k)}_{sym}$. Moreover

$$\mathbf{\hat{U}}_{k+1}' := (\mathbf{U}_{k}' \otimes U) \cap \mathcal{S}(\mathbf{U}_{k}' \otimes U) \subset (\mathbf{U}_{k} \otimes U) \cap \mathcal{S}(\mathbf{U}_{k} \otimes U) = \mathbf{\hat{U}}_{k+1}$$

guarantees the existence of a subspace $\mathbf{U}'_{k+1} \subset \hat{\mathbf{U}}'_{k+1}$ so that the construction can be continued. However, may it happen that \mathbf{U}'_k is too small and $\hat{\mathbf{U}}'_{k+1} = \{0\}$ holds?

8 Combination with ANOVA

As already mentioned in [9, $\S17.4.4$] the ANOVA⁷ representation has favourable properties in connection with symmetric tensors. The ANOVA technique is briefly described in $\S8.1$ (see also Bohn–Griebel [4, $\S4.3$]). The ANOVA approximation uses terms with low-dimensional minimal subspaces. Therefore the combination with the TT format is an efficient approach.

⁷ANOVA abbreviates 'analysis of variance'.

8.1 ANOVA Technique

Let $0 \neq e \in V$ be a special element. In the case of multivariate functions, e may be the constant function e(x) = 1. In the case of mappings, e is the identity mapping. Define

$$E := \operatorname{span}\{e\}, \qquad \mathring{V} := E^{\perp}. \tag{8.1}$$

The choice of the orthogonal complement E^{\perp} simplifies later computations. Theoretically, it would be sufficient to choose \mathring{V} such that there is a direct sum

$$V = E \oplus \mathring{V}.$$

The space \mathring{V} gives rise to the symmetric tensor space $\mathring{\mathbf{V}}_{sym}^{(d)}$.

We introduce the following notation of symmetric tensors in $\mathbf{V}_{\text{sym}}^{(d)}$ generated by tensors from $\mathbf{\mathring{V}}_{\text{sym}}^{(k)}$:

$$S(\mathbf{v};d) := \mathcal{S}_d(\mathbf{v} \otimes (\otimes^{d-k} e)) \qquad \text{for } \mathbf{v} \in \mathring{\mathbf{V}}_{\text{sym}}^{(k)} \text{ with } 1 \le k \le d.$$
(8.2)

The tensors in (8.2) form the following subspaces of $\mathbf{V}_{\text{svm}}^{(d)}$:

$$\mathbf{\mathring{V}}_0 := \otimes^d E, \qquad \mathbf{\mathring{V}}_k := \mathcal{S}_d(\mathbf{\mathring{V}}_{sym}^{(k)} \otimes (\otimes^{d-k} E)) \quad \text{for } 1 \le k \le d.$$

Lemma 8.1 If (8.1) holds, there is an orthogonal decomposition $\mathbf{V}_{\text{sym}}^{(d)} = \bigoplus_{j=0}^{d} \mathbf{\mathring{V}}_{j}$.

Proof. Let $k > \ell$, $\mathbf{v} \in \mathring{\mathbf{V}}_k$, $\mathbf{w} \in \mathring{\mathbf{V}}_\ell$. Tensor \mathbf{v} can be written as a sum of elementary tensors $\mathbf{v}_{\nu} = \bigotimes_{j=0}^d v_{\nu}^{(j)}$ containing k vectors $v_{\nu}^{(j)} \in \mathring{V}$. Correspondingly, \mathbf{w} is a sum of $\mathbf{w}_{\mu} = \bigotimes_{j=0}^d w_{\mu}^{(j)}$ with $d - \ell$ vectors $w_{\mu}^{(j)} = e$. Because of $\ell < k$, there must be some j with $v_{\nu}^{(j)} \in \mathring{V}$ orthogonal to $w_{\mu}^{(j)} = e$. Hence $\langle \mathbf{v}_{\nu}, \mathbf{w}_{\mu} \rangle = 0$ holds for all pairs implying $\langle \mathbf{v}, \mathbf{w} \rangle = 0$.

The ANOVA representation of a (symmetric) tensor $\mathbf{v} \in \mathbf{V}_{sym}^{(d)}$ is the sum

$$\mathbf{v} = \sum_{k=0}^{L} \mathbf{v}_k \qquad \text{with } \mathbf{v}_k \in \mathring{\mathbf{V}}_k \text{ for some } 0 \le L \le d.$$
(8.3)

We call L the ANOVA degree.

Remark 8.2 (a) The motivation of ANOVA is to obtain an approximation (8.3) for a relative small degree L.

(b) Let $\mathbf{v}_{ex} = \sum_{k=0}^{d} \mathbf{v}_k$ be the exact tensor. In order to approximate \mathbf{v}_{ex} by \mathbf{v} from (8.3) we have to assume that the terms \mathbf{v}_k are (rapidly) decreasing.

8.2 Representation

We assume that (8.3) holds with $\mathbf{v}_k = S(\mathbf{x}_k; d)$. The tensors $\mathbf{x}_k \in \mathring{\mathbf{V}}_{sym}^{(k)}$ are given together with their minimal subspaces $\mathbf{U}_k^{\min}(\mathbf{x}_k)$ as described in §5.5.

We generalise the notation $S(\cdot; d)$ in (8.2) to subspaces:

$$S(\mathbf{X}; d) = \operatorname{span}\{S(\mathbf{x}; d) : \mathbf{x} \in \mathbf{X}\} \text{ for } \mathbf{X} \subset \check{\mathbf{V}}_{\operatorname{sym}}^{(k)}.$$

If $\mathbf{X} = \operatorname{span}\{\mathbf{x}_{\nu} : 1 \leq \nu \leq N\}$, we have $S(\mathbf{X}; d) = \operatorname{span}\{S(\mathbf{x}_{\nu}; d) : 1 \leq \nu \leq N\}$. We remark that $\mathbf{U}_{d}^{\min}(\mathbf{v}) = \operatorname{span}\{\mathbf{v}\}$ for $\mathbf{v} \in \otimes^{d} V$.

Lemma 8.3 Let $\mathbf{v}_k \in \mathring{\mathbf{V}}_k$. Then

$$U_{j}^{\min}(S(\mathbf{v}_{k};d)) = \sum_{\mu=\min\{j,k-j\}}^{\max\{k,d-j\}} S(U_{\mu}^{\min}(\mathbf{v}_{k});j).$$
(8.4)

Proof. By definition of $U_{j-k}^{\min}(\cdot)$, functionals in d-j directions are to be applied. Let μ be associated with \mathbf{v}_k and $d-j-\mu$ with $\otimes^{d-k} e$. This leads to the inequalities $0 \le \mu \le k$ and $0 \le d-j-\mu \le d-k$. Together they imply $\min\{j, k-j\} \le \mu \le \max\{k, d-j\}$.

Consider the case of j = d - 1. Applying φ with $\varphi(e) = 1$ and $\varphi(v) = 0$ ($v \in \mathring{V}$), we obtain $\varphi^{(d)}(S(\mathbf{v}_k;d)) = S(\mathbf{v}_k;d-1)$, provided that k < d. On the other hand, φ with $\varphi(e) = 0$ yields $\varphi^{(d)}(S(\mathbf{v}_k;d)) = S(\varphi(\mathbf{v}_k);d-1)$. This proves

$$\mathbf{U}_{d-1}^{\min}(S(\mathbf{v}_k;d)) = S(\mathbf{v}_k;d-1) + S(\mathbf{U}_{k-1}^{\min}(\mathbf{v}_k);d-1).$$

Since span{ $S(\mathbf{v}_k; d-1)$ } = $S(\mathbf{U}_k^{\min}(\mathbf{v}_k); d-1)$, this coincides with (8.4) for j = d-1. For the other j apply Remark 1.5 recursively.

The ANOVA tensor is the sum $\mathbf{v} = \sum_k \mathbf{v}_k$. As $\mathbf{U}_j^{\min}(\mathbf{a} + \mathbf{b}) \subset \mathbf{U}_j^{\min}(\mathbf{a}) + \mathbf{U}_j^{\min}(\mathbf{b})$, we obtain from (8.4) that

$$\mathbf{U}_{j}^{\min}\left(S\left(\sum_{k}\mathbf{v}_{k};d\right)\right)\subset\sum_{k,\mu}S(\mathbf{U}_{\mu}^{\min}(\mathbf{v}_{k});j).$$

The dimension of the right-hand side may be larger than $\mathbf{U}_{j}^{\min}(\mathbf{v})$, but here we want to separate the spaces E and $\hat{U} \subset \hat{V}$. For instance, the tensor $\mathbf{v} = (a+e) \otimes (a+e)$ has the one-dimensional minimal subspace $U_{1}^{\min}(\mathbf{v}) = \operatorname{span}\{a+e\}$, but here we use $E + \hat{U}$ with $\hat{U} = \operatorname{span}\{a\}$.

8.3 Example

Consider an expression of the form $\sum_{i} S(a'_{i}; d) + S(\mathbf{b}; d)$, where $a'_{i} \in V$ and $\mathbf{b} \in \mathbf{V}_{sym}^{(2)}$. We assume that \mathbf{b} can be approximated by $\sum_{k} (b'_{k} \otimes c'_{k} + c'_{k} \otimes b'_{k})$. Orthogonalisation of a'_{i}, b'_{k}, c'_{k} with respect to some e yields the vectors a_{i}, b_{k}, c_{k} and the ANOVA form

$$\mathbf{v} = \alpha S(1; d) + \sum_{i=1}^{N_1} S(x_i; d) + \sum_{k=1}^{N_2} S(a_k \otimes b_k + b_k \otimes a_k; d),$$
(8.5)

where x_i represents a_i and multiples of b_k and c_k . Note that $S(1;d) = \otimes^d e$. In the following we give the details for

 $\mathbf{v} = \alpha S(1; d) + S(x; d) + S(a \otimes b + b \otimes a; d).$

The combined ANOVA-TT format uses the spaces

$$j = 1 : U_{1} = \operatorname{span}\{e, x, a, b\},$$

$$j = 2 : \mathbf{U}_{2} = \operatorname{span}\{S(1; 2), S(x; 2), S(a; 2), S(b; 2), S(a \otimes b + b \otimes a, 2)\},$$

$$\vdots$$

$$j < d : \mathbf{U}_{j} = \operatorname{span}\{S(1; j), S(x; j), S(a; j), S(b; j), S(a \otimes b + b \otimes a, j)\},$$

$$j = d : \mathbf{U}_{d} = \operatorname{span}\{\mathbf{v}\}.$$
(8.6)

The essential recursive definition (5.3) of the basis reads as follows:

$$\begin{split} S(1;j) &= S(1;j-1) \otimes e, \\ S(x;j) &= S(x;j-1) \otimes e + S(1;j-1) \otimes x, \\ S(a;j), \ S(b;j): \ \text{analogously,} \\ S(a \otimes b + b \otimes a,j) &= S(a \otimes b + b \otimes a,j-1) \otimes e \\ &+ S(a;j-1) \otimes b + S(b;j-1) \otimes a. \end{split}$$

The final step follows from

$$\mathbf{v} = \alpha S(1; d-1) + S(x; d-1) \otimes e + S(1; d-1) \otimes x + S(a \otimes b + b \otimes a, d-1) \otimes e + S(a; d-1) \otimes b + S(b; d-1) \otimes a.$$

Remark 8.4 The terms

$$\alpha S(1;d)$$
 and $\sum_{k=1}^{N_2} S(a_k \otimes b_k + b_k \otimes a_k;d)$

in (8.5) lead to $3N_2 + 1$ basis vectors in \mathbf{U}_j . Let N_0 vectors x_i be linearly independent of span $\{a_k, b_k : 1 \le k \le N_2\}$. Then $\sum_{i=1}^{N_1} S(x_i; d)$ requires N_0 additional basis vectors in \mathbf{U}_j .

8.4 Operations

Concerning scalar product one can exploit Lemma 8.1: $\langle S(\mathbf{v}; d), S(\mathbf{w}; d) \rangle = 0$ for $\mathbf{v} \in \mathring{\mathbf{V}}_k$, $\mathbf{w} \in \mathring{\mathbf{V}}_\ell$ with $k \neq \ell$. If the basis of \mathbf{U}_j should be orthonormalised, it is sufficient to orthonormalise only the contributions $S(\mathbf{v}_{\nu}; j)$ for all $\mathbf{v}_{\nu} \in \mathring{\mathbf{V}}_k$ separately (cf. (8.6)).

One can possibly use that for tensors $\mathbf{v}_{\nu}, \mathbf{w}_{\nu} \in \mathbf{V}_k, k \leq j$, the scalar product $\langle S(\mathbf{v}; j), S(\mathbf{w}; j) \rangle$ is a fixed multiple of $\langle \mathbf{v}, \mathbf{w} \rangle$, provided that $\langle e, e \rangle = 1$:

$$\langle S(\mathbf{v};j), S(\mathbf{w};j) \rangle = \frac{j!}{k!} \langle \mathbf{v}, \mathbf{w} \rangle.$$

In principle, the operations within the TT format are as usual. However, one has to take care that the result is again of the ANOVA form.

As an example we consider the Hadamard product \odot (pointwise product) for multivariate functions. For the standard choice that e is the constant function with value 1, we have $e \odot e = e$ (and $a \odot e = e \odot a = a$ for any a). If \mathbf{v} is of the form (8.3) with $L = L_v$, while \mathbf{w} corresponds to $L = L_w$, the product $\mathbf{z} := \mathbf{v} \odot \mathbf{w}$ satisfies (8.3) with degree $L_z = \min\{d, L_v + L_w\}$. Enlarging L increases the storage cost and the arithmetic cost of operations involving \mathbf{z} . A truncation $L_z \mapsto L'_z < L_z$ could be helpful, provided that omitted terms are small. Here we need that \mathbf{z} satisfies the assumption of Remark 8.2b.

Let Z = L(V) be the space of linear maps of V into V. Another example is the multiplication of an operator (Kronecker matrix) $\mathbf{A} = \sum_{k=0}^{L_A} \mathbf{A}_k \in \mathbf{Z}_{sym}^{(d)}$ and a tensor $\mathbf{v} = \sum_{k=0}^{L_v} \mathbf{v}_k \in \mathbf{V}_{sym}^{(d)}$. Let the identity be the special element I of Z (replacing e in the general description). This guarantees Ie = e. Again $\mathbf{w} := \mathbf{A}\mathbf{v}$ is of the form (8.3) with $L_w = \min\{d, L_A + L_v\}$. Only under the assumption that all maps in $U_1^{\min}(\mathbf{A})$ possess e as an eigenvector, we have $L_w = L_v$.

9 Operators, Kronecker Matrices

If V is a matrix space, the corresponding tensor space contains Kronecker matrices. More generally, linear operators on multivariate functions can be described by tensors. In this case, there is an operator \mathbf{A} and a vector \mathbf{v} as well as the product $\mathbf{A}\mathbf{v}$. For completeness we list the relations between (anti)symmetric operators and (anti)symmetric tensors \mathbf{v} . The proofs are obvious and therefore omitted.

The expression $\pi \mathbf{A}$ used below means the application of the permutation π to the tensor $\mathbf{A} \in \otimes^d L(V) \subset L(\mathbf{V})$, where L(V) are the linear maps from V into itself. Concerning $\otimes^d L(V) \subset L(\mathbf{V})$ compare [9, Proposition 3.49].

Lemma 9.1 Let $\mathbf{V} = \otimes^d V$, $\mathbf{A} : \mathbf{V} \to \mathbf{V}$ a linear map and π a permutation. Then the action of $\pi \mathbf{A}$ can be expressed by the action of \mathbf{A} :

$$(\pi \mathbf{A}) \mathbf{u} = \pi \left(\mathbf{A} \left(\pi^{-1} \mathbf{u} \right) \right) \quad \text{for all } \mathbf{u} \in \mathbf{V}.$$

If **A** is symmetric then $\pi(\mathbf{A}\mathbf{u}) = \mathbf{A}(\pi\mathbf{u})$. If $\mathbf{u} \in \mathbf{V}_{sym}$ then $(\mathcal{S}(\mathbf{A}))\mathbf{u} = \mathcal{S}(\mathbf{A}\mathbf{u})$. If $\mathbf{A} : \mathbf{V} \to \mathbf{V}$ is symmetric then $\mathbf{A}\mathcal{S}(\mathbf{u}) = \mathcal{S}(\mathbf{A}\mathbf{u})$.

The last statement implies that if $\mathbf{A} : \mathbf{V} \to \mathbf{V}$ is symmetric, then $\mathbf{A} : \mathbf{V}_{sym} \to \mathbf{V}_{sym}$ and $\mathbf{A} : \mathbf{V}_{anti} \to \mathbf{V}_{anti}$.

The adjoint of **A** is denoted by \mathbf{A}^* , i.e., $\langle \mathbf{A}\mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{u}, \mathbf{A}^*\mathbf{v} \rangle$. Any permutation satisfies $\pi^* = \pi^{-1}$ and $(\pi \mathbf{A})^* = \pi \mathbf{A}^*$. In particular, permutations of selfadjoint operators are again selfadjoint.

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