Constrained Tensor Product Approximations based on Penalized Best Approximations

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Abstract

In this paper, we propose some alternative definitions of tensor product approximations based on the progressive construction of successive best rank-one approximations, with eventual updates of previously computed elements. In particular, it can be interpreted as a constrained multidimensional singular value decomposition where the constraints are imposed by means a penalty method. A convergence proof of these decompositions is established under some general assumptions on the penalty functional. Heuristic alternated direction algorithms are provided, also definitions and algorithms are detailed for an application of interest consisting in imposing bounds on each tensor component.

Key words: Tensor product approximation; Constrained Separated Representation; Penalization; Convex optimization; Constrained Singular Value decomposition; Proper Generalized Decomposition

1. Introduction

Tensor product approximation has become a major tool in many domains of scientific computing for the representation of elements in high-dimensional tensor product spaces. It consists in approximating an element u of a tensor product space $V = V_1 \otimes \ldots \otimes V_d$ by a sum of elementary tensors

$$u \approx u_m = \sum_{i=1}^{m} w_i^1 \otimes \ldots \otimes w_i^d$$

with $w_i^k \in V_k$. The dimensionality of this type of representation only grows linearly with the dimension d and therefore, it allows to circumvent the so

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[1] Supported by the French National Research Agency (grant SIM-DREAM).

called curse of dimensionality. A first family of applications using tensor decompositions concerns the extraction of information from complex data. It has been used in many areas such as psychometrics [28, 6], chemometrics [3], analysis of turbulent flows [4], image analysis and pattern recognition [30], data mining... Another family of applications concerns the compression of complex data (for storage or transmission), also introduced in many areas such as signal processing [19] or computer vision [31]. A survey of tensor decompositions in multilinear algebra and an overview of possible applications can be found in the review paper [17]. In the above applications, the aim is to compress the best as possible the information or to extract a few modes representing some features to be analyzed. The use of tensor product approximation is also receiving a growing interest in numerical analysis for the solution of problems defined in high-dimensional tensor product spaces, such as PDEs arising in stochastic calculus [2, 5, 12] (e.g. Fokker-Planck equation), stochastic parametric PDEs arising in uncertainty quantification with spectral approaches [21, 11, 22]. In the context of approximation, the aim is to represent the tensor with a given accuracy, without necessarily requiring an optimal compression of the tensor.

Many definitions of tensor product approximations have been proposed. A natural definition of a rank-m tensor product approximation is based on the following best approximation problem

$$\inf_{u_m \in \mathcal{S}_m} \|u - u_m\|^2 \tag{1}$$

where $\|\cdot\|$ is the norm on V and $\mathcal{S}_m$ is an optimization subset of rank-m tensors. For dimension $d = 2$, and when $\|\cdot\|$ is a crossnorm on a tensor product Hilbert space V [14], this definition coincides with the classical truncated singular value decomposition of u, also called Proper Orthogonal Decomposition or Karhunen-Loeve expansion in other contexts. For $d \geq 3$, optimization problem (1) appears to be ill-posed [9] if formulated on the whole set of rank-m tensors. This specificity has led to the introduction of various definitions of tensor product approximations based on different choices for the optimization sets $\mathcal{S}_m$ [29]. They can be considered as multidimensional versions of the singular value decomposition.

In this paper, we propose alternative definitions for tensor product approximations based on successive rank-one best approximations, with eventual updates of previously constructed elements. The main contribution consists in introducing a methodology for constructing tensor product approximation of tensors submitted to additional constraints. The question is: how to modify the classical definitions of tensor product approximations in order to have an approximation which still verifies the constraints or at least which verifies the constraints "better" than classical tensor product approximations ? We propose to impose the constraints approximately with a penalty method which consists

in defining the decomposition u_m with a modified best approximation problem

$$\inf_{u_m \in \mathcal{S}_m} \frac{1}{2}\|u - u_m\|^2 + j_\epsilon(u_m) \tag{2}$$

where j_ϵ is a penalty function associated with the constraints, with suitable properties ensuring the existence of a minimizer. An application of interest which will be detailed and illustrated concerns the case where we want the components of the approximation to be bounded (upper, lower or lower and upper bounded). Let us consider the case where V is a set of functions $u : \Omega \to \mathbb{R}$ defined on a cartesian domain $\Omega = \Omega_1 \times \ldots \times \Omega_d \subset \mathbb{R}^d$, and consider a function u which is bounded by two constants a and b, i.e. $a \leq u(x) \leq b$. Classical tensor product approximations do not guaranty that this property is preserved for a truncated approximation u_m. Moreover, for general functions u, we may not have a uniform convergence of u_m, which means that we can not expect to verify the constraint (almost) everywhere for a given finite rank m. However, preserving the boundedness properties may be of great importance in some situations. For example, let us consider a diffusion problem $-\nabla \cdot (u(x)\nabla p(x)) = f(x)$, where u denotes the diffusion parameter field. In order to apply efficiently solution techniques based on tensor product approximation of the solution p, the diffusion operator must be approximated in a separated form. It consists in replacing u by a tensor product approximation u_m. However, it requires to verify $0 < a \leq u(x) \leq b < \infty$ almost everywhere in order to preserve the well-posedness of the diffusion equation.

The outline of the paper is as follows. In section 2, we briefly recall some definitions about tensor product spaces in infinite and finite dimensional Hilbert spaces. In section 3, we recall classical definitions of tensor product approximations and we detail definitions based on progressive constructions of best rank-one approximations, with eventual updates of previously computed elements. In section 4, we introduce new definitions of constrained tensor product approximations based on a penalty method and we propose algorithms for their constructions. Convergence proof of the decompositions are given under some assumptions on the penalty function. In section 5, we apply the previous definitions to the case where we want to impose bounds on tensor product approximations. An illustration is given for the separated representation of the indicator function of a three-dimensional object. A possible application concerns the coupling of tensor product solvers with fictitious domain formulations for the solution of PDEs [23, 25].

2. Tensor product spaces

2.1. Tensor product of Hilbert spaces

We consider Hilbert spaces V_k, $1 \leq k \leq d$, equipped with inner products $(\cdot,\cdot)_k$ and associated norms $\|\cdot\|_k$. We define the set of elementary tensors (or rank-one tensors)

$$\mathcal{R}_1 = \{w = w^1 \otimes \ldots \otimes w^d; w^k \in V_k, 1 \leq k \leq d\}$$

and the set of rank-m tensors

$$\mathcal{R}_m = \{v_m = \sum_{i=1}^{m} w_i; w_i \in \mathcal{R}_1, 1 \leq i \leq m\} = \mathcal{R}_{m-1} + \mathcal{R}_1$$

The algebraic tensor product space is defined as the span of elementary tensors

$$_a\otimes_{k=1}^{d} V_k = \text{span}\{\mathcal{R}_1\}$$

For each element $v \in {}_a\otimes_{k=1}^{d} V_k$, there exists $m \in \mathbb{N}$ such that $v \in \mathcal{R}_m$. The algebraic tensor product space is now equipped with the canonical inner product $(\cdot,\cdot)$ defined as follows. For elementary tensors $w = \otimes_{k=1}^{d} w^k \in \mathcal{R}_1$ and $v = \otimes_{k=1}^{d} v^k \in \mathcal{R}_1$, we let

$$(w, v) = (\otimes_{k=1}^{d} w^k, \otimes_{k=1}^{d} v^k) = \prod_{k=1}^{d} (w^k, v^k)_k$$

This definition is then extended by linearity on the whole algebraic tensor product space: for $w, v \in {}_a\otimes_{k=1}^{d} V_k$, there exists $m, m' \in \mathbb{N}$ such that $w = \sum_{i=1}^{m} \otimes_{k=1}^{d} w_i^k$ and $v = \sum_{i=1}^{m'} \otimes_{k=1}^{d} v_i^k$, and the inner product (v, w) is defined by

$$(v, w) = \sum_{i=1}^{m}\sum_{j=1}^{m'} (\otimes_{k=1}^{d} w_i^k, \otimes_{k=1}^{d} v_j^k) = \sum_{i=1}^{m}\sum_{j=1}^{m'}\prod_{k=1}^{d} (w_i^k, v_j^k)_k$$

The norm associated with $(\cdot,\cdot)$ is denoted $\|\cdot\|$. For an elementary tensor $w = \otimes_{k=1}^{d} w^k \in \mathcal{R}_1$, the norm verifies

$$\| \otimes_{k=1}^{d} w^k \| = \prod_{k=1}^{d} \|w^k\|_k$$

which is the property of a crossnorm. The algebraic tensor product space ${}_a\otimes_{k=1}^{d} V_k$ is a pre-Hilbert space when equipped with inner product $(\cdot,\cdot)$. A Hilbert space V equipped with inner product $(\cdot,\cdot)$ and associated norm $\|\cdot\|$ is obtained by the completion of the algebraic tensor product space

$$V = \overline{{}_a\otimes_{k=1}^{d} V_k}^{\|\cdot\|}$$

We have the following important topological property of the set of rank-one tensors (see [13] for a proof).

Lemma 2.1. *The set $\mathcal{R}_1$ is weakly closed in V.*

Let us note that equivalent norms induce the same topology on V. Therefore, for any topology associated with a norm equivalent to a crossnorm, the set $\mathcal{R}_1$ is also weakly closed. The connection between the choice of norms and the induced topological properties are detailed in [24]. In particular, for the choice of norms leading to a weakly closed set $\mathcal{R}_1$, it is given weaker conditions than the equivalence with a crossnorm.

2.2. Finite dimensional case

In the finite dimensional case, we can assume that $V_k = \mathbb{R}^{n_k}$, up to an isomorphism. An element $w^k \in V_k$ is then represented by a vector $w^k = \sum_{l=1}^{n_k} w_l^k e_l^k \in \mathbb{R}^k$, where the $\{w_l^k\}_{l=1}^{n_k}$ are the components of w^k on the canonical orthonormal basis $\{e_l^k\}_{l=1}^{n_k}$ of $\mathbb{R}^{n_k}$. Each V_k is endowed with the canonical inner product $(\cdot,\cdot)_k$ and associated norm $\|\cdot\|_k$, defined for elementary tensors $w = \otimes_{k=1}^d w^k \in \mathcal{R}_1$ and $v = \otimes_{k=1}^d w^k \in \mathcal{R}_1$ by

$$(w,v) = \prod_{k=1}^{d} (w^k, v^k)_k = \prod_{k=1}^{d} \sum_{l_k=1}^{n_k} w_{l_k}^k v_{l_k}^k, \quad \|w\|^2 = \prod_{k=1}^{d} \|w^k\|_k^2 = \prod_{k=1}^{d} \sum_{l_k=1}^{n_k} (w_{l_k}^k)^2$$

V coincides with the algebraic tensor product space and $V = \text{span}\{\mathcal{R}_1\}$. V is isomorphic to the set of multidimensional arrays $\mathbb{R}^{n_1 \times \ldots \times n_k}$. A tensor $u \in V$ admits a full representation

$$u = \sum_{l_1=1}^{n_1} \ldots \sum_{l_d=1}^{n_d} u_{l_1,\ldots,l_d} e_{l_1}^1 \otimes \ldots \otimes e_{l_d}^d := \sum_{l \in L} u_l e_l$$

where $L = \{(l_1, \ldots, l_d) \in \mathbb{N}^d; 1 \leq l_k \leq n_k\}$ is the set of multi-indices and the $u_l = u_{l_1,\ldots,l_d}$ are the components of u on the canonical basis $\{e_l = \otimes_{k=1}^d e_{l_k}^k\}_{l \in L}$. Components of a rank-1 tensor $w = \otimes_{k=1}^d w^k \in \mathcal{R}_1$ are

$$w_{l_1,\ldots,l_d} = w_{l_1}^1 \ldots w_{l_d}^d$$

Components of a rank-m tensor $u = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes w_i^d \in \mathcal{R}_m$ are

$$u_{l_1,\ldots,l_d} = \sum_{i=1}^{m} w_{l_1,i}^1 \ldots w_{l_d,i}^d$$

For $u, v \in V$, the above definitions yield the following classical definition of the canonical inner product and associated norm on V:

$$(u,v) = \sum_{l_1=1}^{n_1} \ldots \sum_{l_d=1}^{n_d} u_{l_1,\ldots,l_d} v_{l_1,\ldots,l_d}, \quad \|u\|^2 = \sum_{l_1=1}^{n_1} \ldots \sum_{l_d=1}^{n_d} (u_{l_1,\ldots,l_d})^2$$

In the case of finite dimensional Hilbert spaces, all norms induce the same topological vector space V, and therefore, Lemma 2.1 implies that $\mathcal{R}_1$ is a closed set in V, whatever the choice of norm.

Lemma 2.2. *For a finite dimensional tensor product Hilbert space V, the set $\mathcal{R}_1$ is closed in V.*

3. Tensor product approximations

An optimal rank-m representation of $u \in V$ could be naturally defined by the following best approximation problem:

$$\inf_{v_m \in \mathcal{R}_m} \|u - v_m\|^2 \tag{3}$$

For $d = 2$, it leads to a classical singular value decomposition of u, truncated at rank m. However, for $d \geq 3$, $\mathcal{R}_m$ is not weakly closed in V, even in the finite dimensional case [9]. Therefore, the minimization problem (3) is ill-posed since a minimizer in $\mathcal{R}_m$ does not necessarily exist. A "less optimal" but well posed rank-m approximation u_m can be defined by

$$\|u - u_m\|^2 = \min_{v_m \in \mathcal{S}_m \subset \mathcal{R}_m} \|u - v_m\|^2 \tag{4}$$

where $\mathcal{S}_m$ is a suitable subset in $\mathcal{R}_m$ which ensures the existence of a minimizer. Of course, depending on the choice of $\mathcal{S}_m$, different types of decompositions arise. In this section, we recall some classical definitions and investigate different alternative definitions which lead to well posed definitions of the approximation.

3.1. Tensors sets with orthogonality constraints

The set $\mathcal{S}_m$ can be defined by imposing suitable orthogonality conditions between rank-1 tensors of the decomposition of a rank-m tensor. Let $w = \otimes_{k=1}^d w^k$ and $v = \otimes_{k=1}^d v^k$ be two rank-one tensors. We define different types of orthogonality:

- Orthogonality: w and v are said orthogonal if and only if $(w, v) = \prod_{k=1}^d (w^k, v^k)_k = 0$. It is denoted $w \perp v$.
- Strong orthogonality: w and v are said strongly orthogonal if and only if $w \perp v$ and for all $k \in \{1, \ldots, d\}$, we have either $(w^k, v^k)_k = 0$ or $w^k = \lambda^k v^k$ for some $\lambda^k \in \mathbb{R}$. It is denoted $w \perp_s v$.
- Complete orthogonality: w and v are said completely orthogonal if and only if $(w^k, v^k) = 0$ for all $k \in \{1, \ldots, d\}$. It is denoted $w \perp_c v$.

To the above definitions of orthogonality, we associate different subsets of rank-m tensors:

- $\mathcal{R}_m^{\perp} = \{\sum_{i=1}^m w_i \in \mathcal{R}_m; w_i \perp w_j \text{ for } i \neq j\}$
- $\mathcal{R}_m^{\perp_s} = \{\sum_{i=1}^m w_i \in \mathcal{R}_m; w_i \perp_s w_j \text{ for } i \neq j\}$
- $\mathcal{R}_m^{\perp_c} = \{\sum_{i=1}^m w_i \in \mathcal{R}_m; w_i \perp_c w_j \text{ for } i \neq j\}$

We have the following inclusions:

$$\mathcal{R}_m^{\perp_c} \subset \mathcal{R}_m^{\perp_s} \subset \mathcal{R}_m^{\perp} \subset \mathcal{R}_m.$$

It is proved in [29] that the best approximation problem (4) admits a minimizer when choosing for $\mathcal{S}_m$ the subsets $\mathcal{R}_m^{\perp_c}$, $\mathcal{R}_m^{\perp_s}$ or $\mathcal{R}_m^{\perp}$. Let us note that for every tensor $u \in V$, there exists a sequence $\{u_m\} \subset \mathcal{R}_m^{\perp}$ or $\{u_m\} \subset \mathcal{R}_m^{\perp_s}$ that converges to u. This is due to the fact that the tensor product space admits a strongly orthogonal Hilbertian basis. However, a tensor $u \in V$ does not necessarily admits a convergent representation $\{u_m\} \subset \mathcal{R}_m^{\perp_c}$. Therefore, complete orthogonality has to be imposed with caution.

Another choice for $\mathcal{S}_m$ consists in taking the Tucker space $\mathcal{T}_{\mathbf{r}}$, with $\mathbf{r} = (r_1, \ldots, r_d) \in \mathbb{N}^d$, defined by

$$\mathcal{T}_{\mathbf{r}} = \left\{ \sum_{i_1=1}^{r_1} \ldots \sum_{i_d=1}^{r_d} \alpha_{i_1,\ldots,i_d} w_{i_1}^1 \otimes \ldots \otimes w_{i_d}^d ; \alpha_{i_1,\ldots,i_d} \in \mathbb{R}, w_i^k \in V_k, (w_i^k, w_j^k)_k = \delta_{ij} \right\} \tag{5}$$

The set $\mathcal{T}_{\mathbf{r}}$ is a weakly closed set in V [15] and therefore, the best approximation problem (4) is also well posed on the set $\mathcal{S}_m = \mathcal{T}_{\mathbf{r}} \subset \mathcal{R}_m$, with $m = \prod_{k=1}^d r_k$. Let us note that we have $\mathcal{R}_1 = \mathcal{T}_{(1,\ldots,1)}$ and $\mathcal{R}_m \subset \mathcal{T}_{(m,\ldots,m)}$.

Remark 3.1. *In the Tucker representation* (5), $\alpha = (\alpha_{i_1,\ldots,i_d}) \in \mathbb{R}^{r_1 \times \ldots \times r_d}$ *is called the core tensor. Let us note that the number of components* $m = \prod_{k=1}^d r_k$ *in the core tensor grows exponentially with* d*, if* $card\{k \in \{1, \ldots, d\}; r_k \geq 2\} \to \infty$ *as* $d \to \infty$.

The reader can refer to [7, 18, 17, 29] for a detailed presentation of the above tensor product approximations and of the related algorithms for their construction. Let us note that other definitions are also available [28, 16].

3.2. Progressive constructions

We here present alternative definitions of rank-m approximations based on the progressive construction of optimal rank-one elements, with eventual updates of the previously computed vectors. Let us note that they can be interpreted as updated Greedy approximations [10, 27] where dictionary is composed by elementary tensors. These definitions appear as particular cases of constrained approximations which are proposed in section 4.

3.2.1. Purely progressive construction

Another way to obtain a well-posed problem (4) is to construct the approximation progressively. Knowing an approximation $u_{m-1} \in \mathcal{R}_{m-1}$, we define the set

$$\mathcal{S}_m = u_{m-1} + \mathcal{R}_1 \subset \mathcal{R}_m.$$

Since $\mathcal{R}_1$ is a weakly closed set in V, the above set $\mathcal{S}_m$ is also a weakly closed set and therefore, the best approximation problem (4) is well defined and allows to define a new element $u_m = u_{m-1} + w_m \in \mathcal{R}_m$, where the new rank-one term $w_m \in \mathcal{R}_1$ appears as a best approximation in $\mathcal{R}_1$ of the residual $u - u_{m-1}$. This construction defines a multidimensional version of a singular value decomposition, known in multilinear algebra as the best rank-one decomposition of a tensor [8].

Definition 3.2 (MSVD). *For an element* $u \in V$*, the purely progressive multidimensional singular value decomposition is defined as a sequence of rank-*m *approximations* $u_m = \sum_{i=1}^m w_i \in \mathcal{R}_m$ *defined progressively as follows:*

$$\|u - u_{m-1} - w_m\|^2 = \min_{w \in \mathcal{R}_1} \|u - u_{m-1} - w\|^2 \tag{6}$$

We have the following property:

$$\|u - u_m\|^2 = \|u\|^2 - \sum_{i=1}^{m} \sigma_i^2 \xrightarrow[m\to\infty]{} 0$$

where

$$\sigma_i = \|w_i\| = \max_{w\in\mathcal{R}_1, \|w\|=1} (u - u_{i-1}, w) \tag{7}$$

σ_i can be interpreted as the dominant singular value of $u - u_{i-1}$. For convergence results in infinite dimensional Hilbert spaces, the reader can refer to [13]. Note that this definition of singular value has also been introduced in [20].

Remark 3.3. *The map*

$$\varepsilon : v \in V \mapsto \varepsilon(v) = \max_{w\in\mathcal{R}_1, \|w\|=1} (v, w) \in \mathbb{R}^+$$

is a particular crossnorm called the injective norm [14]. The dominant singular value σ_i defined in (7) then appears to be the injective norm of the residual $u - u_{i-1}$, i.e. $\sigma_i = \varepsilon(u - u_{i-1})$. This interpretation can be found in quantum physics [26].

Remark 3.4. *In the case $d = 2$, Definition 3.2 coincides with the classical singular value decomposition. For $d = 2$, equation (7) writes*

$$\sigma_i = \max_{w^1\otimes w^2\in\mathcal{R}_1, \|w^1\otimes w^2\|=1} (u - u_{i-1}, w^1 \otimes w^2)$$

For $u \in V$ and $w^1 \in V_1$, we define $\{u, w^1\}_1 \in V_2$ such that $(\{u, w^1\}_1, w^2)_2 = (u, w^1 \otimes w^2)$ for all $w^2 \in V_2$. In the same way, for $u \in V$ and $w^2 \in V_2$, we define $\{u, w^2\}_2 \in V_1$ such that $(\{u, w^2\}_2, w^1)_1 = (u, w^1 \otimes w^2)$ for all $w^1 \in V_1$. Next, we define the operators $U : w^1 \in V_1 \mapsto \{u - u_{i-1}, w^1\}_1 \in V_2$ and $U^* : w^2 \in V_2 \mapsto \{u - u_{i-1}, w^2\}_2 \in V_1$. U^* is the adjoint operator of U, i.e. such that $(Uw^1, w^2)_2 = (w^1, U^*w_2)_1$ for all $(w^1, w^2) \in V_1 \times V_2$. The dominant singular value can then be written:

$$\sigma_i = \max_{w^1\in V_1, w^2\in V_2, \|w^1\|_1=1, \|w^2\|_2=1} (Uw^1, w^2)_2$$

After an elimination of w^2, we obtain $w^2 = Uw^1/\|Uw^1\|_2$ and the previous expression becomes:

$$\sigma_i = \max_{w^1\in V_1, \|w^1\|_1=1} \sqrt{(w^1, U^*Uw^1)_1}$$

which is the classical definition of the dominant singular value of operator U, which is the square root of the dominant eigenvalue of operator U^*U. Equivalently, after an elimination of w^1, we obtain $w^1 = U^*w^2/\|U^*w^2\|_1$ and

$$\sigma_i = \max_{w^2\in V_2, \|w^2\|_2=1} \sqrt{(w^2, UU^*w^2)_2}$$

This property motivates the interpretation of Definition 3.2 as a multidimensional version of a singular value decomposition.

Remark 3.5. *Let us note that the progressive construction could be also defined by replacing $\mathcal{R}_1$ by the Tucker space $\mathcal{T}_{\mathbf{r}}$, which is also a weakly closed set in V. A sequence $\{u_m\}_{m\in\mathbb{N}}$ is then defined progressively by letting $u_m = u_{m-1} + z_m$, with $z_m \in \mathcal{T}_{\mathbf{r}}$ defined by*

$$\|u - u_{m-1} - z_m\|^2 = \min_{z\in\mathcal{T}_{\mathbf{r}}} \|u - u_{m-1} - z\|^2$$

We then have $u_m \in \mathcal{T}_{\mathbf{r}^*} \subset \mathcal{R}_{m^*}$, with $\mathbf{r}^* = (mr_1, \ldots, mr_d)$ and $m^* = m^d \prod_{k=1}^d r_k$.

3.2.2. Progressive construction with updates

Convergence properties of the progressive construction can be improved by introducing updates of previously computed tensors. These updates are performed along selected dimensions. Let $D \subset \{1, \ldots, d\}$ be a subset of dimensions. For a given $k \in D$ and a given $u_m = \sum_{i=1}^m \otimes_{k=1}^d w_i^k \in \mathcal{R}_m$, let us introduce the space

$$\mathcal{R}_m^k(u_m) = \left\{ \sum_{i=1}^m w_i^1 \otimes \ldots \otimes v_i^k \otimes \ldots \otimes w_i^d; v_1^k, \ldots, v_m^k \in V_k \right\} \subset \mathcal{R}_m \qquad (8)$$

where vectors $\{w_i^{k'}\}_{i=1}^m$ are fixed for all $k' \neq k$. $\mathcal{R}_m^k(u_m)$ is a linear subspace of $\mathcal{R}_m$. We then define the map

$$F_m^k : u_m \in \mathcal{R}_m \mapsto z_m = F_m^k(u_m) \in \mathcal{R}_m^k(u_m)$$

which updates the vectors $\{w_i^k\}_{i=1}^m$ associated with dimension k. The map is defined as follows:

$$z_m = F_m^k(u_m) \quad \Leftrightarrow \quad \|u - z_m\|^2 = \min_{v_m \in \mathcal{R}_m^k(u_m)} \|u - v_m\|^2 \qquad (9)$$

Note that the minimization problem on $\mathcal{R}_m^k(u_m)$ is ill-posed if the linear subspace $\mathcal{R}_m^k(u_m)$ is not a closed linear subspace of V. If such a degeneracy is detected, we simply let $F_m^k(u_m) = u_m$ (no update performed). Now, for a given set D of updated dimensions, we define the map F_m^D as the composition of maps $\{F_m^k\}_{k\in D}$:

$$F_m^D = F_m^{d_1} \circ \ldots \circ F_m^{d_{\#D}}$$

where we let $D = \{d_1, \ldots, d_{\#D}\}$, with $\#D$ the cardinal of D. Let us note that different orderings of the set D yield different definitions of the map F_m^D.

Definition 3.6 (Updated MSVD). *For an element $u \in V$, the updated progressive multidimensional singular value decomposition is defined as a sequence of rank-m approximations $u_m \in \mathcal{R}_m$ defined progressively as follows: for $u_{m-1} = \sum_{i=1}^{m-1} w_i \in \mathcal{R}_{m-1}$ given, we define $u_m^\diamond \in u_{m-1} + \mathcal{R}_1$ by*

$$\|u - u_m^\diamond\|^2 = \min_{w\in\mathcal{R}_1} \|u - u_{m-1} - w\|^2$$

and we define u_m by applying N_{up} times the updates along a set of dimensions D:

$$u_m = \underbrace{F_m^D \circ \ldots \circ F_m^D}_{N_{up}\ times}(u_m^\diamond)$$

3.2.3. Algorithm

Alternated direction algorithm for minimization in $\mathcal{R}_1$. For a given $u_{m-1} \in \mathcal{R}_{m-1}$, an optimal rank-one element $w_m \in \mathcal{R}_1$, defined by (6), can be constructed with the Alternated Direction Algorithm 1.

Algorithm 1 (Alternated Direction Algorithm).

Initialize $w \in \mathcal{R}_1$ *with* $\|w\| = 1$
loop *{Maximum number of iterations* N_{max}^{alt}*}*
  $w := G_m^d \circ \ldots \circ G_m^1(w)$
  $\sigma := \|w\|$
  $w := w/\sigma$
  Check convergence (on σ*)*
end loop
Set $w_m := \sigma w$

Algorithm 1 involves the application of successive maps $G_m^k : \mathcal{R}_1 \to \mathcal{R}_1$, for $k = 1, \ldots, d$. The application of map G_m^k to an element $w = \otimes_{k=1}^d w^k \in \mathcal{R}_1$ consists in modifying the vector $w^k \in V_k$ by minimizing $\|u - u_{m-1} - \otimes_{l=1}^d w^l\|$ with respect to w^k, letting fixed the other vectors w^l, for $l \neq k$. The map can be defined as follows:

$$z = G_m^k(w) \quad \Leftrightarrow \quad \|u - u_{m-1} - z\|^2 = \min_{z \in \mathcal{R}_1^k(w)} \|u - u_{m-1} - z\|^2$$

where for $w = \otimes_{k=1}^d w^k$, $\mathcal{R}_1^k(w)$ is defined by

$$\mathcal{R}_1^k(w) = \{w^1 \otimes \ldots \otimes v^k \otimes \ldots \otimes w^d; v^k \in V_k\} \subset \mathcal{R}_1, \tag{10}$$

For $w \neq 0$, $\mathcal{R}_1^k(w)$ is a closed linear subspace of rank-1 tensors, such that the minimization on $\mathcal{R}_1^k(w)$ is always well-posed and admits a unique solution. Therefore, the map G_m^k is well defined. $z = G_m^k(w)$ is equivalently characterized by

$$z \in \mathcal{R}_1^k(w), \quad (z, v) = (u - u_{m-1}, v) \quad \forall v \in \mathcal{R}_1^k(w)$$

Denoting $z = w^1 \otimes \ldots \otimes z^k \otimes \ldots \otimes w^d$, the previous equation is formulated as a problem on $z^k \in V_k$:

$$(z^k, v^k)_k \prod_{l=1, l\neq k}^{d} \|w^l\|_l^2 = (u - u_{m-1}, w^1 \otimes \ldots \otimes v^k \otimes \ldots \otimes w^d) \quad \forall v^k \in V_k$$

from which we deduce the expression of z^k :

$$z^k = \{u - u_{m-1}, w\}_{*k} \prod_{l=1, l\neq k}^{d} \|w^l\|_l^{-2}$$

where for $v \in V$ and $w \in \mathcal{R}_1$, $\{v, w\}_{*k} \in V_k$ is defined by

$$(\{v, w\}_{*k}, v^k)_k = (v, w^1 \otimes \ldots \otimes v^k \otimes \ldots \otimes w^d) \quad \forall v^k \in V_k \tag{11}$$

Finally, the map G_m^k can be simply defined as follows:

$$G_m^k(w) = w^1 \otimes \ldots \otimes g_m^k(w) \otimes \ldots \otimes w^d,$$

with

$$g_m^k(w) = \{u - u_{m-1}, w\}_{*k} \prod_{l=1, l\neq k}^{d} \|w^l\|_l^{-2}$$

Remark 3.7. *Algoritm 1 can be interpreted as a multidimensional extension of a power method for capturing the dominant singular value of a tensor and an associated rank-one tensor (called singular vector), defined by* (7)*. In the case* $d = 2$*, it exactly coincides with a classical power method yielding the dominant singular value and vector defined in Remark 3.4. For* $d > 2$*, this algorithm has already been introduced in multilinear algebra, where it is called Higher Order Power Method [8].*

Algorithm for rank-m approximation. We now propose the following algorithm for the construction of a rank-m tensor product approximation, introduced in Definition 3.6. This algorithm corresponds to a progressive construction with N_{up} updates along selected directions $D \subset \{1, \ldots, d\}$. Let us note that with $N_{up} = 0$, this algorithm allows the construction of the purely progressive MSVD introduced in Definition 3.2.

Algorithm 2 (Progressive construction with updates).

Set $u_0 := 0$
for $i = 1$ *to* m ***do***
  Compute $w_i \in \mathcal{R}_1$ *with Algorithm 1*
  Set $u_i := u_{i-1} + w_i$
  loop *{*N_{up} *times}*
    $u_i := F_i^D(u_i)$
  end loop
end for

We recall that $F_m^D = F_m^{d_1} \circ \ldots \circ F_m^{d_{\#D}}$. Let us now detail for a given $k \in D$ the application of the map F_m^k, defined by (9). Let $u_m = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes w_i^d$. Since $\mathcal{R}_m^k(u_m)$ is a linear subspace, $z_m = F_m^k(u_m)$ is characterized by

$$z_m \in \mathcal{R}_m^k(u_m), \quad (z_m, v_m) = (u, v_m) \quad \forall v_m \in \mathcal{R}_m^k(u_m)$$

Let us denote $z_m = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes z_i^k \otimes \ldots \otimes w_i^d$, with $z_i^k \in V_k$. The previous equation yields the following characterization of the unknown functions $\{z_i^k\}_{i=1}^m \in (V_k)^m$:

$$\sum_{i,j=1}^m \alpha_{ij}(z_j^k, v_i^k)_k = \sum_{i=1}^m (\{u, w_i\}_{*k}, v_i^k)_k \quad \forall v_1^k, \ldots, v_m^k \in V_k,$$

with $\alpha_{ij} = \prod_{l=1,l\neq k}^{d}(w_i^l, w_j^l)_l$. Denoting $\beta \in \mathbb{R}^{m\times m}$ the inverse of matrix $\alpha = (\alpha_{ij}) \in \mathbb{R}^{m\times m}$, we have

$$z_i^k = \sum_{j=1}^{m} \beta_{ij}\{u, w_j\}_{*k} := f_{i,m}^k(u_m) \quad \forall i \in \{1, \ldots, m\}$$

We then have the following expression of map F_m^k:

$$F_m^k(u_m) = \sum_{i=1}^{m} w_i^1 \otimes \ldots \otimes f_{i,m}^k(u_m) \otimes \ldots \otimes w_i^d$$

Let us note that if we have a complete orthogonality between rank-one elements, i.e. $w_i \perp_c w_j$, then α is a diagonal matrix and the map is well defined. For general non orthogonal elements, a degeneracy of the linear space $\mathcal{R}_m^k(u_m)$ may occur, which leads to a singular (or ill-conditioned) matrix α. When such a degeneracy occurs, the update along dimension k is omitted, letting $F_m^k(u_m) = u_m$.

4. Constrained multidimensional tensor product approximation

In this section, we propose a modification of tensor product approximations proposed in section 3 in order to satisfy some desired constraints. The aim is to impose to finite-rank approximations u_m of u to stay in an admissible set of tensors $K \subset V$ that verify the constraints. In this paper, we propose to enforce the constraints with a penalty method and therefore, the constraints will be verified approximately. We restrict the presentation and the convergence results to the practical case of finite dimensional Hilbert spaces. Under more general assumptions, and following [24], the proposed definitions of constrained approximation could be extended to infinite dimensional Hilbert spaces.

Remark 4.1. *When the function u to be approximated verifies the constraints, i.e. $u \in K$, the proposed definitions allows to construct a sequence u_m which converges to u. A less natural situation which could however be of practical interest, is when $u \notin K$. In this case, the proposed definitions allows to construct a sequence u_m which converges to the best approximation of u in K. Both cases are considered in a unique framework.*

4.1. Set of admissible elements and penalty method

Let us consider that $K \subset V$ is a closed subset of elements which verify some desired constraints. We introduce a functional $j : V \to \mathbb{R}^+$ such that

$$\begin{cases} j(v) = 0 & \text{if } v \in K \\ j(v) > 0 & \text{if } v \notin K \end{cases}$$

Assumption 4.2. *Functional $j : V \to \mathbb{R}^+$ is chosen such that:*

(i) j is convex and coercive ($j(v) \to \infty$ as $\|v\| \to \infty$)

(ii) j is Fréchet differentiable, with continuous Fréchet differential $j' : V \to V$.

We now introduce a penalty functional $j_\epsilon : V \to \mathbb{R}^+$ defined by

$$j_\epsilon(v) = \epsilon j(v)$$

with $\epsilon > 0$ a penalty parameter, and we introduce a functional $J_\epsilon : V \to \mathbb{R}$ defined by

$$J_\epsilon(v) = \frac{1}{2}\|u - v\|^2 + j_\epsilon(v) \tag{12}$$

A suitable subset $A \subset V$ being given, a best approximation $u_\epsilon^A \in A$ of $u \in V$ which verifies approximately the constraints can then be defined by the optimization problem

$$J_\epsilon(u_\epsilon^A) = \min_{v \in A} J_\epsilon(v) \tag{13}$$

Let us note that for $\epsilon = 0$, u_0^A is the classical best approximation of u in A, with respect to norm $\|\cdot\|$. Letting $\epsilon \to \infty$, j_ϵ tends towards the characteristic function of the set K and, under suitable assumptions on A, u_ϵ^A tends to the solution u_∞^A of

$$\|u - u_\infty^A\|^2 = \min_{v \in A \cap K} \|u - v\|^2 \tag{14}$$

Increasing ϵ leads to a better verification of the constraints. We have the following properties of functional J_ϵ.

Lemma 4.3. *Functional $J_\epsilon : V \to \mathbb{R}$ defined in (12) verifies*

(i) J_ϵ is positive, strictly convex and coercive

(ii) J_ϵ is continuous and Fréchet differentiable with continuous Fréchet differential $J'_\epsilon : V \to V$ defined by

$$(J'_\epsilon(v), w) = (v - u, w) + (j'_\epsilon(v), w) \quad \forall w \in V$$

Proof. We have $J_\epsilon(v) = J_0(v) + j_\epsilon(v)$, with $J_0(v) = \frac{1}{2}\|u - v\|^2$. In a finite dimensional Hilbert space V, J_0 is a continuous coercive and strictly convex function. J_ϵ is then the sum of a convex coercive and positive functional j_ϵ and of a strictly convex positive and coercive functional J_0. Therefore, J_ϵ is strictly convex, coercive and positive, which proves (i). Next, as a sum of two Fréchet differentiable functionals, J_ϵ is Fréchet differentiable. The continuity of J'_ϵ follows from the assumed continuity of j'_ϵ. That proves (ii). ■

We now recall a classical result in optimization [1] which guaranties the well-posedness of minimization problem (13).

Lemma 4.4. *Let A be a closed subset of a finite dimensional Hilbert space V and let $J : V \to \mathbb{R}$. If J is a convex continuous and coercive functional, it admits a minimizer on A. Moreover, if J is strictly convex, the minimizer is unique.*

We have the following result which characterizes the minimizer of J_ϵ in Hilbert space V.

Proposition 4.5. *The problem*

$$J_\epsilon(u_\epsilon) = \min_{v \in V} J_\epsilon(v) \tag{15}$$

admits a unique solution $u_\epsilon \in V$, equivalently characterized by

$$(J'_\epsilon(u_\epsilon), v) = (u_\epsilon - u, v) + (j'_\epsilon(u_\epsilon), v) = 0 \quad \forall v \in V \tag{16}$$

If $u \in K$ or if $\epsilon = 0$, we have $u_\epsilon = u$.

Proof. The existence of a unique minimizer u_ϵ in the vector space V follows from properties of functional J_ϵ given in Lemma 4.3 and from Lemma 4.4 with an optimization set $A = V$, i.e. the entire Hilbert space. Equation (16) is the classical Euler-Lagrange equation which characterizes the minimizer u_ϵ. Finally, if $u \in K$, we have $J_\epsilon(u) = 0$ and since $J_\epsilon(v) > 0$ for all $v \neq u$, we have that u is the unique minimizer. $\epsilon = 0$ corresponds to the case without the penalty term. It is then a trivial best approximation problem with respect to norm $\|\cdot\|$, which admits as a unique solution the function u itself. ■

4.2. Constrained tensor product approximations

Optimal constrained tensor product approximations u_m could be defined by

$$J_\epsilon(u_m) = \min_{v_m \in \mathcal{S}_m} J_\epsilon(v_m) \tag{17}$$

with a suitable choice of finite rank tensors sets $\mathcal{S}_m$ ensuring the existence of a minimizer. In particular, the different choices of section 3.1 could be adopted and yield different constrained tensor product approximations. Dedicated algorithms should then be derived for their construction. Here, we propose definitions of constrained finite rank approximations based on the progressive construction of optimal rank-one tensors, with eventual updates of the previously computed vectors. The definitions are natural extensions of definitions of section 3.2, with a modification of the functional to minimize.

4.2.1. Purely progressive construction

We first propose a purely progressive construction of the tensor product approximation.

Definition 4.6 (C_ϵMSVD). *We define the purely progressive constrained multidimensional singular value decomposition of a tensor $u \in V$ as the sequence $u_m = \sum_{i=1}^m w_i \in \mathcal{R}_m$ defined progressively by*

$$J_\epsilon(u_{m-1} + w_m) = \min_{w \in \mathcal{R}_1} J_\epsilon(u_{m-1} + w) \tag{18}$$

The minimization problem (18) can also be written $J_\epsilon(u_m) = \min_{v_m \in \mathcal{S}_m} J_\epsilon(v_m)$ with $\mathcal{S}_m = u_{m-1} + \mathcal{R}_1$. From Lemma 2.2, we have that $\mathcal{S}_m$ is a closed set. Therefore, from Lemma 4.4 and properties of J_ϵ, this minimization problem admits a solution and a sequence $\{u_m\}_{m\in\mathbb{N}}$ exists. The convergence of this sequence is proved in section 4.3.

4.2.2. Progressive construction with eventual updates

Following the construction of section 3.2.2, we now propose to include some updates in the previous progressive construction. We denote by $D = \{d_1, \ldots, d_{\#D}\}$ a set of dimensions. For a given dimension $k \in D$, we define the map $F_m^k : u_m \in \mathcal{R}_m \mapsto F_m^k(u_m) \in \mathcal{R}_m^k(u_m)$, with $\mathcal{R}_m^k(u_m) \subset \mathcal{R}_m$ defined by (8) and

$$z_m = F_m^k(u_m) \quad \Leftrightarrow \quad J_\epsilon(z_m) = \min_{v_m \in \mathcal{R}_m^k(u_m)} J_\epsilon(v_m) \tag{19}$$

Such as in section 3.2.2, if for a given $k \in D$ and a given $u_m \in \mathcal{R}_m$, the set $\mathcal{R}_m^k(u_m)$ is not a closed linear space, $F_m^k(u_m)$ is not defined and we simply let $F_m^k(u_m) = u_m$ (no update performed). Next, we define the updating map $F_m^D : \mathcal{R}_m \to \mathcal{R}_m$ as the composition of the maps $\{F_m^k\}_{k\in D}$:

$$F_m^D = F_m^{d_1} \circ \ldots \circ F_m^{d_{\#D}} \tag{20}$$

We now introduce the following definition.

Definition 4.7 (Updated C$_\epsilon$MSVD). *For an element $u \in V$, the updated progressive constrained multidimensional singular value decomposition is defined as a sequence of rank-m approximations $u_m \in \mathcal{R}_m$ defined progressively as follows: for $u_{m-1} = \sum_{i=1}^{m-1} w_i$ given, we define $u_m^\diamond \in u_{m-1} + \mathcal{R}_1$ by*

$$J_\epsilon(u_m^\diamond) = \min_{w\in\mathcal{R}_1} J_\epsilon(u_{m-1} + w) \tag{21}$$

and we define u_m by applying N_{up} times the updates along a set of dimensions D:

$$u_m = \underbrace{F_m^D \circ \ldots \circ F_m^D}_{N_{up}\ times}(u_m^\diamond)$$

The convergence of the sequence $\{u_m\}_{m\in\mathbb{N}}$ is proved in the following section 4.3.

Remark 4.8. *Let us note that for $\epsilon = 0$, Definition 4.7 (resp. 4.6) coincides with the Definition 3.6 (resp. 3.2) of the unconstrained multidimensional singular value decomposition.*

4.3. Convergence result

Here, we give a convergence proof of the updated progressive tensor product approximation with constraints $\{u_m\}_{m\in\mathbb{N}}$ defined in Definition 4.7. The convergence of the purely progressive construction of Definition 4.6 is obtained as a corollary since it is a particular case of the updated progressive construction

(with $N_{up} = 0$). Let us also note that a convergence result for unconstrained decompositions (Definitions 3.2 and 3.6) is obtained as a corollary of the present result since unconstrained decompositions are particular cases of constrained decompositions, with $\epsilon = 0$ (see remark 4.8). For the definition of the sequence $\{u_m\}_{m\in\mathbb{N}}$, Definition 4.7 introduce an auxiliary sequence $u_m^\diamond$. In the case where no update is performed, we let $u_m = u_m^\diamond$.

Theorem 4.9 (Convergence). *The sequence $\{u_m\}_{m\in\mathbb{N}}$, defined in Definition 4.7, converges towards the unique minimizer u_ϵ of J_ϵ defined in Proposition 4.5:*

$$\|u_\epsilon - u_m\| \xrightarrow[m\to\infty]{} 0$$

Proof. $\{J_\epsilon(u_m)\}_{m\geq 1}$ is a non-increasing sequence. Indeed, by definition,

$$J_\epsilon(u_m) \leq J_\epsilon(u_m^\diamond) = J_\epsilon(u_{m-1} + w_m) \leq J_\epsilon(u_{m-1} + w) \quad \forall w \in \mathcal{R}_1$$

and in particular, we have $J_\epsilon(u_m) \leq J_\epsilon(u_{m-1})$. If there exists m such that $J_\epsilon(u_m) = J_\epsilon(u_{m-1})$, we have $J_\epsilon(u_{m-1}) = \min_{w\in\mathcal{R}_1} J_\epsilon(u_{m-1}+w)$, and by Lemma 4.10, we have that $u_{m-1} = u_\epsilon$, which ends the proof. Let us now suppose that $J_\epsilon(u_m) < J_\epsilon(u_{m-1})$ for all m. $J_\epsilon(u_m)$ is then a strictly decreasing sequence which is bounded below by $J_\epsilon(u_\epsilon)$. Therefore, there exists

$$J^* = \lim_{m\to\infty} J_\epsilon(u_m) \geq J_\epsilon(u_\epsilon) > -\infty.$$

Since J_ϵ is coercive, the sequence $\{u_m\}_{m\in\mathbb{N}}$ is bounded in V. Then, from any subsequence of the initial sequence, we can extract a further subsequence $\{u_{m_k}\}_{k\in\mathbb{N}}$ that converges to some $u^* \in V$. Since J_ϵ is continuous, we have

$$J_\epsilon(u^*) = \lim_{k\to\infty} J_\epsilon(u_{m_k}) = J^*$$

By definition of the sequence $\{u_m\}_{m\in\mathbb{N}}$, we have

$$J_\epsilon(u_{m_{(k+1)}}) \leq J_\epsilon(u_{m_k+1}) \leq J_\epsilon(u_{m_k} + w)$$

for all $w \in \mathcal{R}_1$. Taking the limit with k and by continuity of J_ϵ, we then obtain

$$J_\epsilon(u^*) \leq J_\epsilon(u^* + w) \quad \forall w \in \mathcal{R}_1,$$

Lemma 4.10 then implies that u^* is equal to the minimizer u_ϵ of J_ϵ. We then have that from any subsequence of the initial sequence, we can extract a further subsequence that converges to u_ϵ. It implies that the whole sequence $\{u_m\}_{m\in\mathbb{N}}$ converges to u_ϵ and by the continuity of J_ϵ, we have

$$\lim_{m\to\infty} J_\epsilon(u_m) = J_\epsilon(u_\epsilon)$$

Using the property (24) of J_ϵ in Lemma 4.11, we obtain

$$J_\epsilon(u_m) - J_\epsilon(u_\epsilon) \geq (J_\epsilon'(u_\epsilon), u_m - u_\epsilon) + \frac{1}{2}\|u_\epsilon - u_m\|^2 = \frac{1}{2}\|u_\epsilon - u_m\|^2, \qquad (22)$$

where we have used $J'_\epsilon(u_\epsilon) = 0$. We then obtain

$$\lim_{m\to\infty} \frac{1}{2}\|u_\epsilon - u_m\|^2 \leq \lim_{m\to\infty} J_\epsilon(u_m) - J_\epsilon(u_\epsilon) = 0,$$

which ends the proof. ■

Lemma 4.10. *Let $u^* \in V$ satisfying*

$$J_\epsilon(u^*) = \min_{w\in\mathcal{R}_1} J_\epsilon(u^* + w). \tag{23}$$

Then u^* is the unique minimizer u_ϵ of J_ϵ on V defined in Proposition 4.5.

Proof. For all $\gamma \in \mathbb{R}^+$ and $w \in \mathcal{R}_1$,

$$J_\epsilon(u^* + \gamma w) \geq J_\epsilon(u^*)$$

and therefore

$$(J'_\epsilon(u^*), w) = \lim_{\gamma\to 0^+} \frac{1}{\gamma}(J_\epsilon(u^* + \gamma w) - J_\epsilon(u^*)) \geq 0$$

Since $-\mathcal{R}_1 = \mathcal{R}_1$, we obtain

$$(J'_\epsilon(u^*), w) \;=\; 0 \quad \forall w \in \mathcal{R}_1,$$

and since $\mathrm{span}(\mathcal{R}_1) = V$, we obtain[2]

$$(J'_\epsilon(u^*), v) = 0 \quad \forall v \in V,$$

and the lemma follows from Proposition 4.5. ■

Lemma 4.11. *Functional J_ϵ verifies the following property: for all $v, w \in V$,*

$$J_\epsilon(v) - J_\epsilon(w) \geq (J'_\epsilon(w), v - w) + \frac{1}{2}\|v - w\|^2 \tag{24}$$

Proof.

$$\begin{aligned}
J_\epsilon(v) - J_\epsilon(w) &= \frac{1}{2}\|u - v\|^2 - \frac{1}{2}\|u - w\|^2 + j_\epsilon(v) - j_\epsilon(w) \\
&\geq \frac{1}{2}\|u - v\|^2 - \frac{1}{2}\|u - w\|^2 + (j'_\epsilon(w), v - w) \quad \text{(by convexity of } j_\epsilon) \\
&= \frac{1}{2}(v, v) - \frac{1}{2}(w, w) - (u, v - w) + (j'_\epsilon(w), v - w) \\
&= \frac{1}{2}(v, v) - \frac{1}{2}(w, w) - (w, v - w) + (w - u, v - w) + (j'_\epsilon(w), v - w) \\
&= \frac{1}{2}\|v - w\|^2 + (J'_\epsilon(w), v - w)
\end{aligned}$$

Let us note that this last property could have been classically deduced from the strong convexity property of J_ϵ:

$$(J'_\epsilon(v) - J'_\epsilon(w), v - w) \geq \|v - w\|^2$$

■

[2] In the infinite dimensional case, we have $\mathrm{span}(\mathcal{R}_1)$ dense in V.

4.4. Algorithm

Alternated direction algorithm for minimization in $\mathcal{R}_1$. For a given u_{m-1}, an optimal rank-one element $w_m \in \mathcal{R}_1$, defined by (18), can be constructed with Alternated Direction Algorithm 1 where for $k \in \{1, \ldots, d\}$, the map $G_m^k : \mathcal{R}_1 \to \mathcal{R}_1$ is defined as follows:

$$z = G_m^k(w) \quad \Leftrightarrow \quad J_\epsilon(u_{m-1} + z) = \min_{z \in \mathcal{R}_1^k(w)} J_\epsilon(u_{m-1} + z)$$

where for $w = \otimes_{k=1}^d w^k$, the linear subspace $\mathcal{R}_1^k(w) \subset \mathcal{R}_1$ is defined by (10). For $w \neq 0$, $\mathcal{R}_1^k(w)$ is a closed linear subspace, such that the minimization of J_ϵ on $\mathcal{R}_1^k(w)$ is well-posed and admits a unique solution. Therefore, the map G_m^k is well defined. $z = G_m^k(w) \in \mathcal{R}_1^k(w)$ is characterized by

$$(J'_\epsilon(u_{m-1} + z), v) = 0 \quad \forall v \in \mathcal{R}_1^k(w)$$

or equivalently by

$$(z, v) + (j'_\epsilon(u_{m-1} + z), v) = (u - u_{m-1}, v) \quad \forall v \in \mathcal{R}_1^k(w)$$

Denoting $z = w^1 \otimes \ldots \otimes z^k \otimes \ldots \otimes w^d$, the previous equation yields an equation on $z^k \in V_k$:

$$\alpha z^k + B(z^k) = \{u - u_{m-1}, w\}_{*k} \tag{25}$$

where $\alpha = \prod_{l=1, l \neq k}^d \|w^l\|_l^2$, where $\{\cdot, \cdot\}_{*k} \in V_k$ is defined by (11) and where $B : V_k \to V_k$ is a nonlinear map defined by

$$B(z^k) = \{j'_\epsilon(u_{m-1} + w^1 \otimes \ldots \otimes z^k \otimes \ldots \otimes w^d), w\}_{*k}$$

Nonlinear map B, as the differential of a convex functional, is a monotone map. Equation (25) is a nonlinear equation which admits a unique solution.

Remark 4.12. *In practice, if we further assume the differentiability of j'_ϵ, and therefore of the map B, we can use a Newton iteration solver for the solution of* (25).

Algorithm for rank-m approximation. For the construction of a rank-m tensor product approximation, defined in Definition 4.7, we use Algorithm 2. With $N_{up} = 0$, this algorithm allows the construction of the purely progressive decomposition introduced in Definition 4.6. Mapping F_m^D is defined in (20) as the composition of maps F_m^k, defined in (19). Let us detail the application of map F_m^k for a given $k \in D$. Let $u_m = \sum_{i=1}^m w_i = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes w_i^d$. Since $\mathcal{R}_m^k(u_m)$ is a linear subspace, $z_m = F_m^k(u_m)$ is characterized by

$$z_m \in \mathcal{R}_m^k(u_m), \quad (z_m, v_m) + (j'_\epsilon(z_m), v_m) = (u, v_m) \quad \forall v_m \in \mathcal{R}_m^k(u_m)$$

Let us denote $z_m = \sum_{i=1}^m w_i^1 \otimes \ldots \otimes z_i^k \otimes \ldots \otimes w_i^d$, with $z_i^k \in V_k$. The previous equation is equivalent to the following system of nonlinear equations defining the unknown functions $\{z_i^k\}_{i=1}^m \in (V_k)^m$:

$$\sum_{j=1}^{m} \alpha_{ij} z_j^k + B_i(z_1^k, \ldots, z_m^k) = \{u, w_i\}_{*k} \tag{26}$$

where $\alpha_{ij} = \prod_{l=1, l\neq k}^d (w_i^l, w_j^l)_l$ and where $B_i : (V_k)^m \to V_k$ is a nonlinear map defined by

$$B_i(z_1^k, \ldots, z_m^k) = \left\{ j'_\epsilon(\sum_{j=1}^{m} w_j^1 \otimes \ldots \otimes z_j^k \otimes \ldots \otimes w_j^d), w_i \right\}_{*k}$$

Remark 4.13. *In practice, if we further assume the differentiability of j'_ϵ, and therefore of the maps B_i, we can use a Newton iteration solver for the solution of* (26).

5. Application to the construction of bounded tensor product approximations

We here introduce the application of interest mentioned in the introduction, for imposing bounds on tensor product approximations.

5.1. A continuous point of view

Let V be a space of functions $u : \Omega \to \mathbb{R}$ defined on a cartesian domain $\Omega = \Omega_1 \times \ldots \times \Omega_d$. Let us denote by K the admissible set of functions, defined by

$$K = \{v \in V; a(x) \leq v(x) \leq b(x), x \in \Omega\} \tag{27}$$

We can introduce the convex functional

$$j(v) = \int_\Omega f(v(x); x) dx \tag{28}$$

with $f(\cdot; x) : \mathbb{R} \to \mathbb{R}$ a convex and continuously differentiable function defined by

$$f(y; x) = [a(x) - y]_+^2 + [y - b(x)]_+^2 \tag{29}$$

where $[y]_+ = \max\{0, y\}$ denotes the positive part of y. We have $j(v) = 0$ for $v \in K$ and $j(v) > 0$ for $v \notin K$. Letting $\epsilon \to \infty$, $j_\epsilon = \epsilon j$ tends towards the indicator function of K. Let us note that f is chosen such that j is two times differentiable, which allows the derivation of specific algorithms for the solution of optimization problem (e.g. Newton solver) associated with the construction of the constrained tensor product approximation.

Remark 5.1. *If the constraint has to be imposed only on a subdomain $\widetilde{\Omega} \subset \Omega$, we define the set of admissible functions*

$$K = \{v \in V; a(x) \leq v(x) \leq b(x), x \in \widetilde{\Omega} \subset \Omega\} \tag{30}$$

and we can simply modify the functional f as follows

$$f(y;x) = ([a(x) - y]_+^2 + [y - b(x)]_+^2) I_{\widetilde{\Omega}}(x), \tag{31}$$

where $I_{\widetilde{\Omega}}(x) = 1$ if $x \in \widetilde{\Omega}$ and $I_{\widetilde{\Omega}}(x) = 0$ if $x \notin \widetilde{\Omega}$. If we want to impose only an upper or a lower bound, we can choose:

- $K = \{u; a(x) \leq u(x), x \in \widetilde{\Omega} \subset \Omega\}$ *and* $f(y;x) = [a(x) - y]_+^2 I_{\widetilde{\Omega}}(x)$
- $K = \{u; u(x) \leq b(x), x \in \widetilde{\Omega} \subset \Omega\}$ *and* $f(y;x) = [y - b(x)]_+^2 I_{\widetilde{\Omega}}(x)$

In practice, the above problem will be discretized and recasted in an algebraic form, with $V = \mathbb{R}^{n_1 \times \ldots \times n_d}$. A tensor $u \in V$ is written $u = \sum_{l \in L} u_l e_l$, using the notations of section 2.2. In the previous context of functions defined on a domain Ω, the components u_l can represent the value of the function at some interpolation points $\{x_l\}_{l \in L}$ of a grid contained in domain Ω. The problem is then reformulated in an algebraic setting as follows.

5.2. Algebraic setting

We consider $V = \mathbb{R}^{n_1 \times \ldots \times n_d} \simeq \mathbb{R}^{n_1} \otimes \ldots \otimes \mathbb{R}^{n_d}$. A tensor $u \in V$ is written $u = \sum_{l \in L} u_l e_l$, with the notations of section 2.2. We consider the set K of admissible tensors:

$$K = \{u \in V; a_l \leq u_l \leq b_l, l \in L\} \tag{32}$$

where $a, b \in V$. Functional j can be chosen as follows

$$j(v) = \sum_{l \in L} f(u_l; l) = \sum_{l_1=1}^{n_1} \ldots \sum_{l_d=1}^{n_d} f(u_{l_1,\ldots,l_d}; l_1, \ldots, l_d)$$

where for $l \in L$, $f(\cdot; l) : \mathbb{R} \to \mathbb{R}$ is defined by

$$f(y;l) = [a_l - y]_+^2 + [y - b_l]_+^2 \tag{33}$$

Remark 5.2. *If we want to impose some bounds only on components u_l with l belonging to a subset of indices $\tilde{L} \subset L$, we can use*

$$f(y;l) = ([a_l - y]_+^2 + [y - b_l]_+^2) I_{\tilde{L}}(l), \tag{34}$$

where $I_{\tilde{L}} : L \to \{0, 1\}$ is the indicator function of the set $\tilde{L}$ defined by $I_{\tilde{L}}(l) = 1$ if $l \in \tilde{L}$ and 0 if $l \notin \tilde{L}$.

Functional j admits the differential $j' : V \to V$ defined by

$$(j'(u), v) = \sum_{l \in L} f'(u_l; l) v_l$$

with

$$f'(y; l) = -2[a_l - y]_+ + 2[y - b_l]_+$$

Functional j' admits a differential $j'' : V \to (V \to V)$ defined for $u, v, w \in V$ by

$$(j''(u)(w), v) = \sum_{l \in L} f''(u_l; l) w_l v_l$$

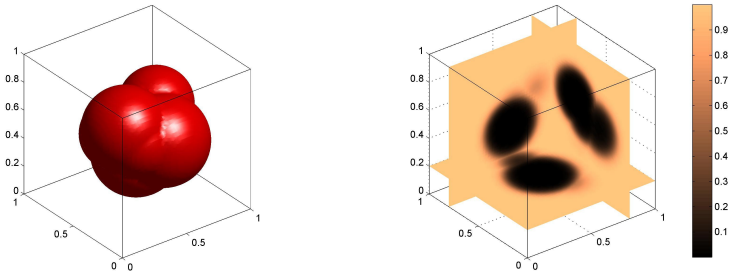
with

$$f''(y; l) = 2H(a_l - y) + 2H(y - b_l)$$

where H is the heaviside function.

5.3. Example: separated representation of the indicator function of a domain

We consider the indicator function $I : (0,1)^3 \to \{0,1\}$ of the three-dimensional domain $\mathcal{O} \subset (0,1)^3$ plotted on figure 1(a). We denote by $\phi : (0,1)^3 \to \mathbb{R}$ the associated level-set function, whose iso-zero is the boundary $\partial\mathcal{O}$. We then introduce a smoothed version $\tilde{I}$ of I defined by $\tilde{I} = \tanh(30\phi)$, plotted in figure 1(b). Finally, we introduce the tensor $u \in \mathbb{R}^{n+1} \otimes \mathbb{R}^{n+1} \otimes \mathbb{R}^{n+1}$ representing the values of $\tilde{I}$ on a cartesian uniform grid in $(0,1)^3$, with $u_{ijk} = \tilde{I}(\frac{i-1}{n}, \frac{j-1}{n}, \frac{k-1}{n})$ for $1 \leq i, j, k \leq n+1$. We here want to find a separated representation u_m of u which verifies $0 \leq u_m \leq 1$. Separated representations are computed with Algo-



(a) (b)

Figure 1: Domain $\mathcal{O}$ (a) and slices of its smoothed indicator function $\tilde{I}$

rithm 2 with a set of updated dimensions $D = \{1, 2, 3\}$. For the construction of rank-1 elements, we use Algorithm 1 with a random initialization, $N_{max}^{alt} = 20$ and a convergence criterium of 10^{-2} (stagnation criterium on σ). In the case of the constrained approximation, the applications of maps G_m^k and F_m^k require the solutions of nonlinear equations (25) and (26), which are solved with a relative precision of 10^{-5} with a Newton solver.

Unconstrained approximation. We first construct an unconstrained multidimensional singular value decomposition (MSVD). Figure 2 shows the convergence of u_m for different numbers N_{up} of updates. We observe that performing one update allows to significantly improve the convergence. However, additional updates does not bring a significant further improvement. Figures 3 plots the

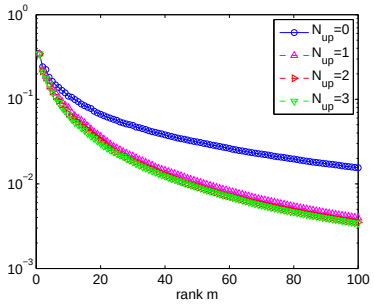


Figure 2: Influence of the number of updates N_{up} in MSVD

maximum and minimum values of u_m. We observe that $u_m \notin (0, 1)$, even for high rank m.

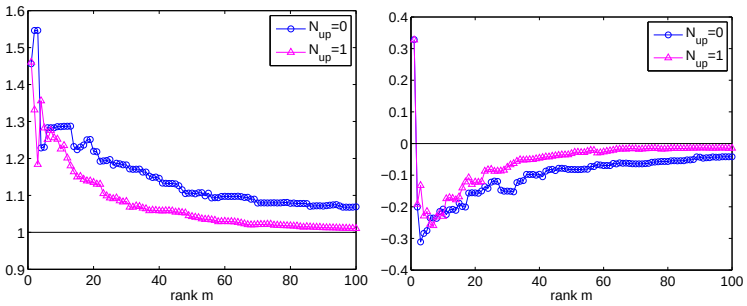
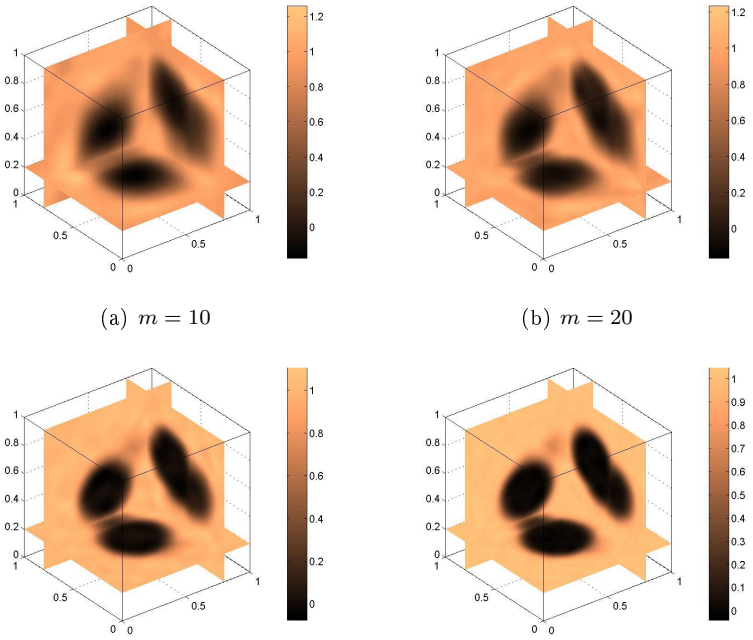


Figure 3: MSVD: minimum (left) and maximum (right) values of u_m for $N_{up} = 0$ and $N_{up} = 1$.

Figure 4 illustrates the obtained approximations u_m for different rank m.



(a) $m = 10$ (b) $m = 20$

(c) $m = 50$ (d) $m = 100$

Figure 4: MSVD: slices of u_m for different m ($N_{up} = 0$).

Constrained approximation. We now construct a constrained multidimensional singular value decomposition (C_ϵMSVD). We consider different values of the penalization parameter $\epsilon \in \{0, 10^{-3}, 10^{-1}, 10^{1}, 10^{3}\}$. We first consider the C_ϵMSVD without updates. Figure 5 illustrates the convergence of associated decompositions u_m, while Figure 6 plots the minimum and maximum values of these decompositions. Figure 7 illustrates slices of decompositions u_m for different values of ϵ. We observe that when ϵ is increased, the convergence rate deteriorates but the constraint is better and better verified. Note that with $\epsilon \leq 10^{-1}$, the obtained decomposition is very close to the unconstrained MSVD. We now

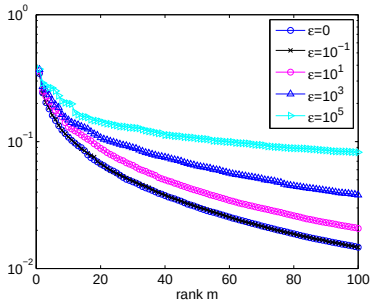


Figure 5: C_ϵMSVD: Convergence of u_m for different values of ϵ.

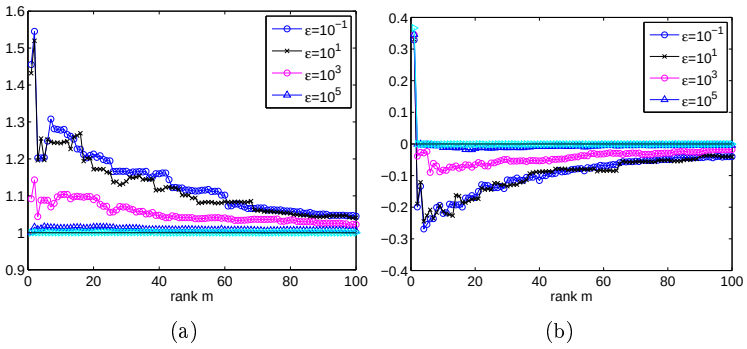
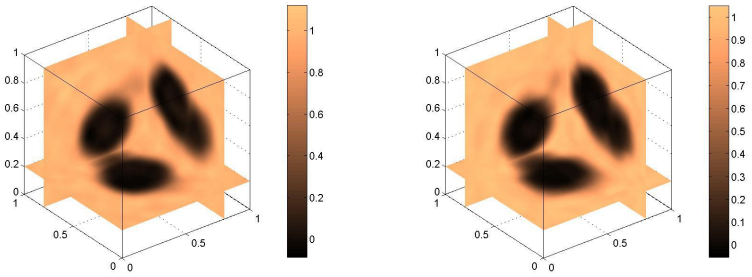


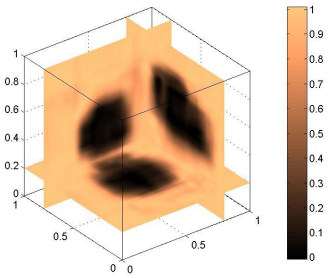
Figure 6: C_ϵMSVD: Minimum (a) and Maximum (b) values of u_m for different ϵ.

improve the constrained decomposition by performing one update ($N_{up} = 1$). Figure 8 illustrates the convergence of this decomposition for $\epsilon = 10^3$. Figure 9 illustrates the minimum and maximum values of constrained decompositions associated with different ϵ. Figure 10 illustrates slices of u_m for $m = 40$ and $\epsilon = 10^3$. Performing one update significantly improved the accuracy for a given rank of decomposition, while preserving the same precision on the verification of the constraint. With one update in the constrained decomposition associated with $\epsilon = 10^3$, we are able to construct a separated representation having the same accuracy than the unconstrained progressive separated representation,

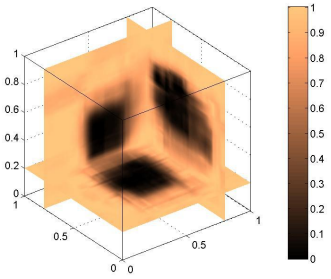


(a) $\epsilon = 10^{-1}$, $m = 40$

(b) $\epsilon = 10^{1}$, $m = 40$



(c) $\epsilon = 10^{3}$, $m = 40$



(d) $\epsilon = 10^{5}$, $m = 40$

Figure 7: C$_\epsilon$MSVD : slices of u_m for different values of penalization parameter ϵ.

with a very good verification of the constraint.

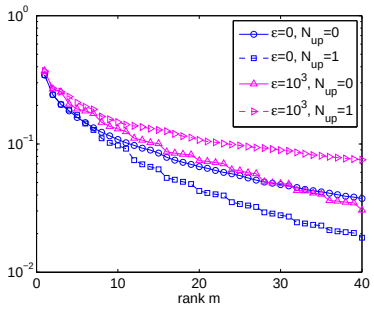
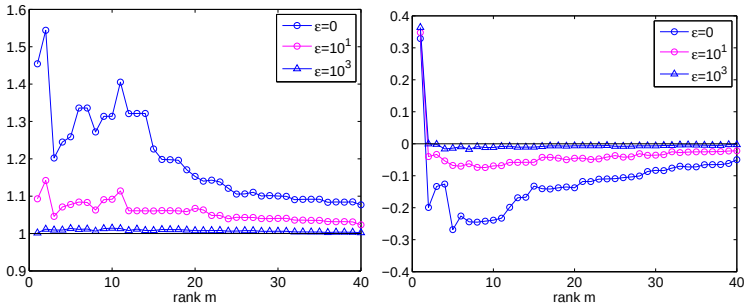
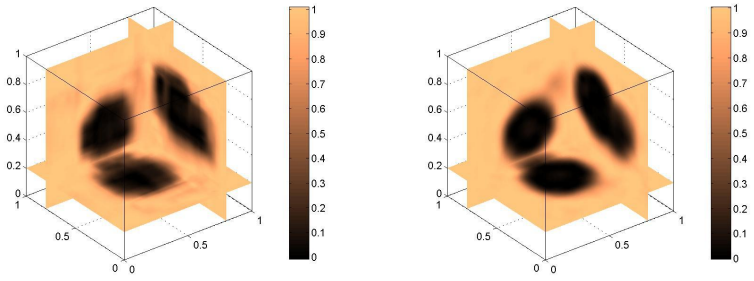


Figure 8: C$_\epsilon$MSVD with updates: convergence of u_m for $\epsilon = 10^3$ and $\epsilon = 0$ (unconstrained decomposition). Influence of updates.



(a) (b)

Figure 9: C$_\epsilon$MSVD with updates: Minimum (a) and Maximum (b) values of u_m for different ϵ, and $N_{up} = 1$.



(a) $\epsilon = 10^3$, $N_{up} = 0$ (b) $\epsilon = 10^3$, $N_{up} = 1$

Figure 10: C$_\epsilon$MSVD : slices of u_m for $m = 40$ and $\epsilon = 10^3$ and for different N_{up}.

6. Conclusion

In this paper, we have proposed some definitions of tensor product approximations based on the progressive construction (eventually updated) of successive best rank-one approximations. In particular, we have proposed new definitions of constrained tensor product approximations based on penalty methods, which allow to enforce some desired constraints on the obtained approximation. The obtained decompositions can be interpreted as constrained multidimensional singular value decomposition. A convergence proof of the tensor product approximations has been established under some natural assumptions on penalty functionals. Heuristic alternated direction algorithms have been provided in order to construct these decompositions. The method has been detailed for the enforcing of bounds on the components of a tensor. The method has been validated on a numerical example.
The results of the present paper have illustrated the feasibility of imposing approximately some constraints on tensor product approximations. However, with the proposed definitions, imposing accurately the constraints may yield a significant deterioration of the convergence properties of the decompositions. Further works should be devoted to alternative definitions allowing to impose the constraints more accurately without a significant deterioration of the convergence. Efficient solution techniques should also be introduced in order to deal with high dimensional tensors. Indeed, the proposed algorithms leads to relatively high computational times for the computation of constrained decompositions. In the case where the initial tensor is given in a separated form, the proposed algorithms for the constrained decomposition uses a full representation of the initial tensor. Therefore, it does not allow to deal with really high dimensional tensor product spaces. In the case where we want to impose bounds on the tensors components, specific algorithms should be introduced in order to perform operations (e.g. positive part, heaviside) preserving the separated form.

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