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MODEL REDUCTION THROUGH MULTILINEAR SINGULAR VALUE DECOMPOSITIONS

Siep Weiland* **and Femke van Belzen***

*Department of Electrical Engineering
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven
The Netherlands.
E-mail: s.weiland@tue.nl

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Abstract. *This paper considers the problem of optimal rank approximations of multilinear functions. A new notion of modal singular values is introduced for an arbitrary tensor and it is shown how optimal lower rank approximations of a tensor can be inferred from these singular values, without resorting to orthogonal tensor decompositions. Results in this paper are primarily motivated by the problem to find optimal projection spaces for model reduction purposes. It is shown that the approximation results outperform earlier singular value based techniques of lower rank approximations of tensors.*

1 INTRODUCTION

Spectral decompositions of signals by (infinite) sequences of orthogonal functions underlie many numerical techniques of approximation and are particularly useful for model or signal approximation methods in computational fluid dynamics. A central theme in many reduction frameworks is therefore the construction of an (empirical) orthonormal basis that proves useful for the representation and approximation of signals. Indeed, most techniques of signal and model compression amount to determining a suitable projection space so as to approximate signals and models on a projective manifold. Especially for signals that evolve over higher dimensional domains, the computation of suitable basis functions may be a formidable task, and it is for this reason that we aim to derive more efficient algorithms for the computation of projection spaces for signal and systems.

Singular value decompositions (SVD's) of matrices have proven to be a key algebraic tool in the construction of projection basis for an enormous class of problems in signal and system approximation. As such, the SVD has found widespread applications. Nevertheless, the classical notion of a singular value decomposition is restricted to matrices or linear mappings on finite dimensional vector spaces and does not allow an immediate or obvious generalization to multi-linear mappings. Only few papers have proposed such generalizations [8, 9, 4] with the aim to find lower rank approximations of multi-way arrays. The complexity and importance of this problem is evidenced in e.g. [5, 12, 13, 10].

This paper focuses on the development of a number of singular value concepts that serve to define singular values of multi-linear functionals (tensors). As a main result it is shown that optimal (modal) rank approximations of a tensor can be characterized by (modal) singular values and in terms of suitable projective subspaces in a multilinear space.

The problem to find optimal lower rank tensors is primarily motivated by the question to define empirical orthonormal basis functions on an N-dimensional domain that lead to spectral expansions of signals for which lower rank approximations are optimal. Many model reduction methods in computational fluid dynamics and particularly the method of proper orthogonal decompositions [1, 3, 11, 6] derive reduced order models on the basis of such empirical basis functions.

2 CONCEPTS FROM MULTI-LINEAR ALGEBRA

Let $\mathcal{W}_1, \ldots, \mathcal{W}_N$ be inner product spaces of dimension $\dim(\mathcal{W}_n) = L_n$ and denote by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ the corresponding inner product and norm in $\mathcal{W}_n$. An *order-N tensor* on the inner product spaces $\mathcal{W}_n$, $n = 1 \ldots, N$, is a multi-linear functional $T : \mathcal{W}_1 \times \ldots \times \mathcal{W}_N \to \mathbb{R}$. That is, T is a linear functional in each of its N arguments. The set of all order-N tensors becomes a vector space, denoted $\mathcal{W}_1 \otimes \cdots \otimes \mathcal{W}_N$, when equipped with the standard definitions of addition and scalar multiplication:

$$(\alpha T_1 + \beta T_2)(w_1, \ldots, w_N) := \alpha T_1(w_1, \ldots, w_N) + \beta T_2(w_1, \ldots, w_N).$$

For fixed elements $v_n \in \mathcal{W}_n$, $n = 1, \ldots, N$, the functional $T : \mathcal{W}_1 \times \ldots \times \mathcal{W}_N \to \mathbb{R}$ defined by

$$T(w_1, \ldots, w_N) = \langle v_1, w_1 \rangle \cdots \langle v_N, w_N \rangle$$

defines an order-N tensor which will be denoted by $v_1 \otimes \cdots \otimes v_N$. If the collection $\{e_n^{\ell_n}, \ell_n = 1, \ldots, L_n\}$ is a basis of $\mathcal{W}_n$, $1 \leq n \leq N$, then T admits a representation

$$T(w_1, \ldots, w_N) = \sum_{\ell_1=1}^{L_1} \cdots \sum_{\ell_N=1}^{L_N} t_{\ell_1, \ldots, \ell_N} e_1^{\ell_1} \otimes \cdots \otimes e_N^{\ell_N}$$

in which the coefficients are encoded in the N-way array $[[t_{i_1, \ldots, i_N}]] \in \mathbb{R}^{L_1 \times \cdots \times L_N}$. As such, an order-1 tensor is encoded as a vector, an order-2 tensor as a matrix, and an order-N tensor as an N-way array.

The *matrix unfolding* of a tensor T is a matrix representation of an N-way array $[[t_{\ell_1, \ldots, \ell_N}]] \in \mathbb{R}^{L_1 \times \cdots \times L_N}$ and is defined for each $n = 1, \ldots, N$ by the matrix

$$T_n \in \mathbb{R}^{L_n \times (L_1 \cdots L_{n-1} L_{n+1} \cdots L_N)}$$

that contains on its ℓ_n-th row all elements $t_{\ell_1,\ldots,\ell_n,\ldots\ell_N}$ where ℓ_m ranges from 1 till L_m with $m \neq n$ (the precise ordering of the columns in T_n will prove irrelevant in the sequel). We refer to T_n as the *n-mode unfolding of T*.

To discuss the problem of low rank approximations of tensors, the concept of tensor rank is of crucial importance. This concept is by no means a trivial extension of the usual notion of matrix rank, and has been discussed in quite a number of papers. See, for example, [4, 5, 10, 8, 9].

Definition 2.1 The *rank* of a nonzero tensor T, denoted $\operatorname{rank}(T)$, is the minimum integer R such that T can be decomposed as $T = \sum_{r=1}^{R} v_1^r \otimes \cdots \otimes v_N^r$ for a suitable collection of elements $v_n^r \in \mathcal{W}_n$, $1 \leq n \leq N$, $1 \leq r \leq R$. The *n-mode rank* of a nonzero tensor T, denoted $\operatorname{rank}_n(T)$, is the rank of the n-mode unfolding T_n of T. The *modal rank* of T, denoted $\operatorname{modrank}(T)$, is the ordered sequence $(R_1, \ldots, R_N)$ of n-mode ranks $R_n = \operatorname{rank}_n(T)$.

The rank and modal rank are well defined in that there exist unique numbers $R = \operatorname{rank}(T)$ and $R_n = \operatorname{rank}_n(T)$ for any $T \in \mathcal{W}_1 \otimes \ldots \otimes \mathcal{W}_N$. If $N = 2$ we have that $R = R_1 = R_2 = \operatorname{rank}(T)$ and the rank coincides with the usual notion of rank of a matrix. For the general case where $N > 2$, it follows that $\operatorname{rank}_n(T) \leq \operatorname{rank}(T)$ for all n, where strict inequality may actually hold for all n [8].

The *operator norm* of a tensor T is defined by

$$\|T\| := \sup_{w_i \in \mathcal{W}_i,\ \|w_i\|=1} |T(w_1, \ldots, w_N)$$

The *Frobenius norm* of a rank R tensor T is

$$\|T\|_F := \inf \left\{ \sum_{r=1}^{R} \|v_1^r\| \cdots \|v_N^r\| \mid T = \sum_{r=1}^{R} v_1^r \otimes \cdots \otimes v_N^r \right\}$$

where $v_n^r \in \mathcal{W}_n$ assumes the norm $\|v_n^r\|$ induced by the inner product in $\mathcal{W}_n$. It is well known that

$$\|T\|_F^2 = \sum_{\ell_1=1}^{L_1} \cdots \sum_{\ell_N=1}^{L_N} t_{\ell_1\ldots\ell_N}^2 = \|[[t_{\ell_1\ldots\ell_N}]]\|_F^2$$

in any basis representation of T.

We associate a number of singular values with an order N tensor as follows.

Definition 2.2 Let $T \in \mathcal{W}_1 \otimes \cdots \otimes \mathcal{W}_N$ be an order-N tensor.

1. The *singular values* of T, denoted $\sigma_k(T)$, with $k = 1, 2, \ldots, K$, with $K = \min_n(L_n)$ are defined recursively as follows:

   - $\mathcal{M}_{n,0} = \mathcal{W}_n$, $1 \leq n \leq N$.

- the kth singular value is

$$\sigma_k(T) = \sup_{w_n \in \mathcal{M}_{n,k-1}, 1 \le n \le N} |T(w_1, \ldots, w_N)| \tag{1}$$

- $\mathcal{M}_{n,k} = \{w_n \in \mathcal{M}_{n,k-1} \mid \langle w_n, w_n^k \rangle = 0\}$ where w_n^k are elements that satisfy $\sigma_k(T) = T(w_1^k, \ldots, w_N^k)$ with $\|w_n^k\| = 1$, $1 \le n \le N$.

2. The *modal singular values* of T, denoted $\sigma_k(T)$, with $k = (k_1, \ldots, k_N)$, $1 \le k_n \le L_n$ are defined as follows

- the $k = (k_1, \ldots, k_N)$th singular value is

$$\sigma_{k_1,\ldots,k_N} = \inf_{\dim \mathcal{L}_n \le L_n - k_n + 1} \sup_{w_n \in \mathcal{L}_n, \|w_n\|=1} T(w_1, \ldots, w_N) \tag{2}$$

- $\mathcal{L}_{n,k_n}$ is the subspace of $\mathcal{W}_n$ of dimension $\dim \mathcal{L}_{n,k_n} \le L_n - k_n + 1$ for which $\sigma_{k_1,\ldots,k_N} = \sup_{w_n \in \mathcal{L}_{n,k_n}, \|w_n\|=1} T(w_1, \ldots, w_N)$

3. The *n-mode singular values* of T are the singular values $\tau_n^1, \ldots, \tau_n^{R_n}$ of the n-mode unfolding T_n of T, i.e., τ_n^i are the elements on the pseudo-diagonal matrix Σ_n in a singular value decomposition $T_n = U_n \Sigma_n V_n^\top$ of T_n.

The definition of n-mode singular values in item 3 has been proposed in [8, 9]. These papers also provide an algorithm for the computation of the n-mode singular values τ_n^i. The concepts in item 1 and 2 are new and have the main advantage that they are defined without reference to a specific basis of the tensor T. Note that we introduced singular values $\sigma_k(T)$ both for integers $k \in \mathbb{N}$ as well as for ordered integer sequences $k \in \mathbb{N}^N$.

The following theorem is the main result of the paper and provides a number of characterizations of the singular values introduced in Definition 2.2.

Theorem 2.3 *Let $T \in \mathcal{W}_1 \otimes \cdots \otimes \mathcal{W}_N$ be an order-N tensor.*

1. $\|T\| = \sigma_1(T) = \sigma_{1,1,\ldots,1}(T)$
2. $\|T\|_F = \sum_{k=1}^K \sigma_k^2(T)$.
3. $\sigma_1(T) \ge \sigma_2(T) \ge \cdots \ge \sigma_K(T)$
4. *For any integer k, $\sigma_{k,k,\ldots,k}(T) \le \sigma_k(T)$*
5. *For all integer k_i we have $\sigma_{k_1,\ldots,k_N}(T) \le \sigma_1(T)$*
6. *If $k_i' \le k_i''$ then $\sigma_{k_1,\ldots,k_i',\ldots,k_N}(T) \le \sigma_{k_1,\ldots,k_i'',\ldots,k_N}(T)$*
7. *For all $n = 1, \ldots, N$ we have the nesting $\mathcal{M}_{n,0} \supset \mathcal{M}_{n,1} \supset \cdots \supset \mathcal{M}_{n,L_n}$.*

8. If $N = 2$ then $\sigma_{k_1,k_2} = \sigma_{k_2,k_1}$,

$$\sigma_{k,k} = \tau_1^k = \tau_2^k = \sigma_k$$

coincides with the kth singular value of the unfolded matrix $T_1 = T_2^\top$ and we have the nesting $\mathcal{L}_{n,1} \supset \cdots \supset \mathcal{L}_{n,L_n}$ for $n = 1, 2$.

The proof of the theorem mainly follows from the definitions. We conjecture that the nesting property in the last item only holds for order-2 tensors and not for higher order tensors. Note also that the last item is simply the 'ordinary' singular value decomposition of the 2-way arrays or matrices $T_1 = T_2^\top$ that is associated with the unfolding of T.

3 LOW RANK APPROXIMATION OF TENSORS

The problem to find a tensor T_r of $\operatorname{rank}(T_r) = r$ such that $\|T - T_r\|$ or $\|T - T_r\|_F$ is generally referred to as the Eckart-Young low rank approximation problem and has been studied in [4, 5, 10, 12]. It was found that lower rank approximations do not need to exist, may not be unique and that the space of rank r tensors is non-compact.

In [8] the authors derive that the approximation error $\|T - T_r\|_F$ is bounded by

$$\|T - T_r\|_F^2 = \sum_{i_1 > r_1} (\tau_1^{i_1})^2 + \cdots + \sum_{i_N > r_N} (\tau_N^{i_N})^2$$

whenever $T_r = T_{r_1,\ldots,r_N}$ is the modal rank $r = (r_1, \ldots, r_N)$ tensor defined by

$$T_{r_1,\ldots,r_N} := \sum_{i_1=1}^{r_1} \cdots \sum_{i_N=1}^{r_N} s_{i_1,\ldots,i_N} \varphi_1^{i_1} \otimes \cdots \otimes \varphi_N^{i_N} \tag{3}$$

where $\varphi_n^{i_n}$, $n = 1, \ldots, N$, $i_n = 1, \ldots, r_n$ denote the i_nth column of U_n in a singular value decomposition $T_n = U_n \Sigma_n V_n^\top$ of the n-mode unfolding T_n of T. It is known that this upperbound may be a strict one. The following result shows that the modal singular values completely characterize the *optimal* modal rank approximations of a tensor in the operator norm.

Theorem 3.1 *For any order-N tensor $T \in \mathcal{W}_1 \otimes \cdots \otimes \mathcal{W}_N$,*

$$\sigma_{r_1+1,\ldots,r_N+1}(T) = \min\{\|T - T_r\| \mid \textit{modrank}\ (T_r) = (r_1, \ldots, r_N)\}.$$

Moreover, an optimal approximant T_r of T is given by (3) if $\varphi_n^{i_n}$ is chosen as an orthonormal basis of the orthogonal complement $\mathcal{L}_{n,r_n+1}^\perp$ of $\mathcal{L}_{n,r_n+1}$ in $\mathcal{W}_n$, $1 \le n \le N$.

Proof: The tensor T_r defined by (3) for the given basis has modal rank $(r_1, \ldots, r_N)$ and has the property that $T_r(w_1, \ldots, w_N) = 0$ whenever $w_n \in \mathcal{L}_{n,r_n+1}$. Since $\mathcal{L}_{n,r_n+1}$ has dimension at most $L_n - r_n$ it follows that

$$\begin{aligned}\sigma_{r_1+1,\ldots,r_N+1}(T) &= \inf_{\dim \mathcal{L}_n \leq L_n - r_n} \sup_{w_n \in \mathcal{L}_n, \|w_n\|=1} T(w_1,\ldots,w_N)\\ &\leq \sup_{w_n \in \mathcal{L}_{n,r_n+1}, \|w_n\|=1} (T - T_r)(w_1,\ldots,w_N)\\ &\leq \sup_{w_n \in \mathcal{W}_n, \|w_n\|=1} |(T - T_r)(w_1,\ldots,w_N)|\\ &= \|T - T_r\|\end{aligned}$$

which shows that $\sigma_{r_1+1,\ldots,r_N+1}(T)$ is a lower bound on the approximation error for any tensor T_r of modal rank $(r_1,\ldots,r_N)$. To show that $\sigma_{r_1+1,\ldots,r_N+1}(T)$ is also an upper-bound for $\|T - T_r\|$, observe that

$$\begin{aligned}\|T - T_r\|^2 &= \|(T - T_r)|_{\mathcal{L}_{1,r_1+1}\times\cdots\mathcal{L}_{N,r_N+1}}\|^2 + \|(T - T_r)|^{\perp}_{\mathcal{L}^{\perp}_{1,r_1+1}\times\cdots\mathcal{L}_{N,r_N+1}}\|^2\\ &= \|T|_{\mathcal{L}_{1,r_1+1}\times\cdots\mathcal{L}_{N,r_N+1}}\|^2 + 0^2\\ &= \sup_{w_n \in \mathcal{L}_{n,r_n+1}, \|w_n\|=1} T(w_1,\ldots,w_N)\\ &= \sigma_{r_1+1,\ldots,r_N+1}(T)\end{aligned}$$

where the last equality follows from the definition of $\mathcal{L}_{n,r_n+1}$. The result then follows. $\square$

Hence, this theorem provides a characterization of the minimal operator norm that can be obtained by approximating T by a lower modal rank tensor in terms of the the modal singular values. Moreover, the result gives an explicit expression for the optimal approximant.

4 APPLICATION IN N-d MODEL REDUCTION

As an application of the results of the previous section, we consider an arbitrary linear N-dimensional system described by the partial differential equation

$$R\left(\frac{\partial}{\partial x_1},\ldots,\frac{\partial}{\partial x_N}\right) w = 0 \tag{4}$$

in which $w : \mathbb{X} \to \mathbb{W}$ evolves over a domain $\mathbb{X} \subset \mathbb{R}^N$ and produces outcomes in a q dimensional real vector space $\mathbb{W} = \mathbb{R}^q$. Here, $R \in \mathbb{R}^{\cdot\times q}[\xi_1,\ldots,\xi_N]$ is a real matrix valued polynomial in N indeterminates. Suppose that the domain $\mathbb{X}$ admits the structure of a Cartesian product $\mathbb{X} = \mathbb{X}_1 \times \ldots \times \mathbb{X}_N$ of N subsets of $\mathbb{R}^N$. A finite element discretization consists of selecting a finite number of functions $\psi_1,\ldots,\psi_L$ in a separable Hilbert space $\mathcal{W}$ in which solutions of (4) reside. Approximate solutions of (4) are then elements w_L of $\mathcal{W}^L = \operatorname{span}\{\psi_1,\ldots,\psi_L\}$ such that the variational expression

$$\langle R\left(\frac{\partial}{\partial x_1},\ldots,\frac{\partial}{\partial x_N}\right) w_L, \psi\rangle_{\mathcal{V}} = 0$$

is satisfied for all $\psi \in \mathcal{W}^L$ where $\mathcal{V}$ is an inner product space contained in $\mathcal{W}$. This method is generally referred to as the *Galerkin projection method*.

Model reduction based on proper orthogonal decomposition (POD) involve empirical basis functions $\{\varphi_\ell, \ell = 1, \ldots, r\}$ of $\mathcal{W}$ (or $\mathcal{W}^L$) that are chosen to minimize the cost function

$$J_r := \sum_{k=1}^{K} \|w^k - \sum_{\ell=1}^{r} \langle w^k, \varphi_\ell \rangle \varphi_\ell\|^2$$

subject to the orthonormality constraint

$$\langle \varphi_i, \varphi_j \rangle = \delta_{i,j}, \quad 1 \leq i, j \leq r$$

where $w^k \in \mathbb{W}$, $1 \leq k \leq K$, is a given ensemble of observations or data and where r denotes the approximation degree. Here, $\| \cdot \|$ denotes the norm induced by the inner product on $\mathcal{W}$.

If $\mathcal{W}$ is finite dimensional, say of dimension L, then a POD basis is given by the left singular vectors in a singular value decomposition of the data ensemble matrix

$$A = \begin{pmatrix} w_1^1 & \cdots & w_1^K \\ \vdots & & \vdots \\ w_L^1 & \cdots & w_L^K \end{pmatrix} = U \Sigma V^\top$$

where w_ℓ^k is the ℓth coefficient of w^k in an arbitrary basis of $\mathcal{W}$, U and V are unitary matrices of dimension $L \times L$ and $K \times K$, respectively, and Σ is a pseudo-diagonal matrix of dimension $L \times K$ with ordered positive numbers $\sigma_1 \geq \cdots \geq \sigma_R$, the *singular values* of A on its main diagonal. Here, $R = \operatorname{rank} A$. In any such decomposition the first r columns $\{\varphi_\ell, \ell = 1, \ldots, r\}$ of U define a POD basis and the minimal value of the cost J_r is given by

$$J_r = \sum_{\ell > r} \sigma_\ell^2.$$

which coincides with the minimal Frobenius norm $\|A - A_r\|_F$ when A_r ranges over all rank r matrices of dimension $L \times K$. Alternatively, the POD basis can be inferred from the normalized eigenvectors corresponding to the r largest eigenvalues of $A^\top A$.

In such a construction, the data ensemble matrix A requires a 'vectorization' of elements in $\mathcal{W}$ in which any possible Cartesian structure that may be present in $\mathbb{X}$ is ignored. Indeed, a finite element discretization of D elements in each of the N coordinates of the spatial domain $\mathbb{X}$ requires a stacking of $L = D^N$ coefficients in the construction of A. Hence the number of rows of A is typically an *exponential function of* N, which may render the calculation of POD bases prohibitive for higher dimensional systems.

Theorem 3.1 provides an N-d spectral expansion of an element $w \in \mathcal{W}$ is an expression of the form

$$w(x_1, \ldots, x_N) = \sum_{\ell_1=1}^{L_1} \cdots \sum_{\ell_N=1}^{L_N} a_{\ell_1 \cdots \ell_N} \varphi_1^{\ell_1}(x_1) \cdots \varphi_N^{\ell_N}(x_N) \tag{5}$$

where $\{\varphi_n^{\ell_n}, \ell_n = 1, \ldots, L_n\}$ are orthonormal basis functions in a Hilbert space $\mathcal{W}_n$ of functions on $\mathbb{X}_n$ and where the coefficients $a_{\ell_1 \cdots \ell_N}$ define an order-N tensor A.

5 CONCLUSIONS

In this paper we proposed a number of definitions of singular values for multilinear functionals (tensor) defined on finite dimensional inner product spaces and derived a number of properties. The notions of singular values that we introduced here are inspired by the minimax property of singual values of matrices, and nicely generalize to multi-linear functions. As a main result it is shown that the minimal error that can be achieved by approximating an order N tensor T by a modal rank $r = (r_1, \ldots, r_N)$ tensors T_r is given by the $(r_1+1, \ldots, r_N+1)$st modal singular value $\sigma_{r_1+1,\ldots,r_N+1}$. This result generalizes the well known relation between lower rank approximations of matrices to arbitrary multilinear functions and improve the error bound in [8, 9] for lower rank approximations of tensors. We derived an analytical expression for the optimal loer rank approximation T_r of T, but we did not yet develop an efficient computational scheme to actually compute T_r. A possible application of the main result in the construction of POD basis function for model reduction purposes has been discussed.

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