

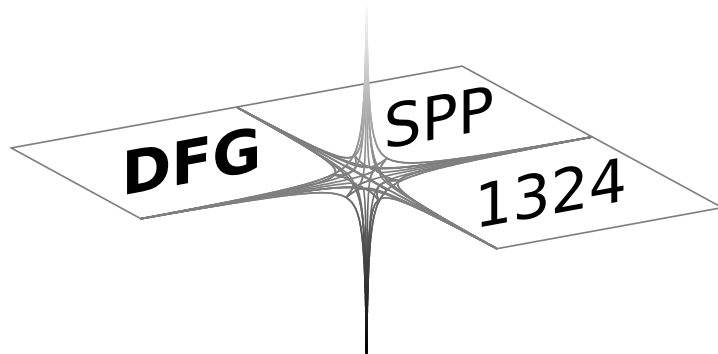
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„Extraktion quantifizierbarer Information aus komplexen Systemen“

Alternating Directions Fitting (ADF) of Hierarchical Low Rank Tensors

L. Grasedyck, M. Kluge, S. Krämer

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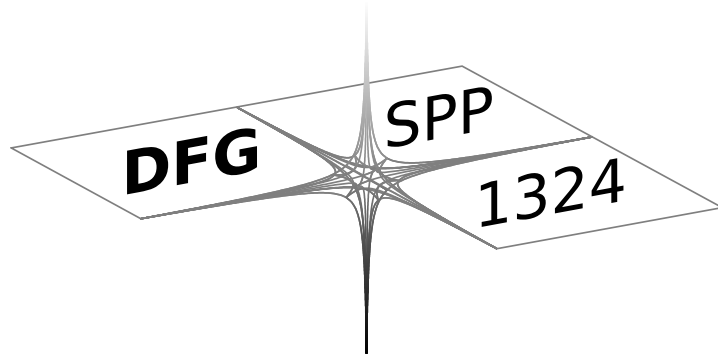
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ALTERNATING DIRECTIONS FITTING (ADF) OF HIERARCHICAL LOW RANK TENSORS

LARS GRASEDYCK*, MELANIE KLUGE* , AND SEBASTIAN KRÄMER*

Abstract. We consider the problem of fitting a low rank tensor $A \in \mathbb{R}^{\mathcal{I}}$, $\mathcal{I} = \{1, \dots, n\}^d$, to a given set of data points $\{M_i \in \mathbb{R} \mid i \in P\}$, $P \subset \mathcal{I}$. The low rank format under consideration is the hierarchical or TT or MPS format. It is characterized by rank bounds r on certain matricizations of the tensor. The number of degrees of freedom is in $\mathcal{O}(dnr^2)$. For a fixed rank and mode size n we observe that it is possible to approximate a tensor from a number of samples that is in $\mathcal{O}(\log N)$ for a tensor having $N = n^d$ entries. Our approach is an alternating directions fitting (ADF) inspired by the LMaFit method for matrix completion, but generalized to tensor completion. We aim at finding a tensor A that fulfils the first order optimality conditions by a nonlinear SOR-type solver that consists of an alternating fit cycling through the directions $\mu = 1, \dots, d$. In the numerical experiments we observe robustness of the completion algorithm with respect to noise and good reconstruction capability. Our tests provide evidence that the algorithm is suitable in higher dimension (>10) as well as for moderate ranks.

Keywords: MPS, Tensor Completion, Tensor Train, TT, Hierarchical Tucker, HT, ALS.
MSC: 15A69, 65F99

1. Introduction. We consider the problem of fitting a low rank tensor

$$A \in \mathbb{R}^{\mathcal{I}}, \quad \mathcal{I} := \mathcal{I}_1 \times \dots \times \mathcal{I}_d, \quad \mathcal{I}_\mu := \{1, \dots, n_\mu\}, \quad \mu \in D := \{1, \dots, d\},$$

to given data points

$$\{M_i \in \mathbb{R} \mid i \in P\}, \quad P \subset \mathcal{I}, \quad \#P \geq \sum_{\mu=1}^d n_\mu,$$

by minimizing the distance between the given values $(M_i)_{i \in P}$ and approximations $(A_i)_{i \in P}$:

$$A = \operatorname{argmin}_{A \in T} \sum_{i \in P} (M_i - \tilde{A}_i)^2 \quad (T \text{ being a certain tensor class})$$

In the class of general dense tensors this is trivial, because the entries of the tensor are all independent. For sparse tensors this reduces to a simple Knapsack problem. Our target tensor class is the set of low rank tensors, i.e., we assume that the implicitly given tensor $M \in \mathbb{R}^{\mathcal{I}}$ allows for a low rank approximation

$$\|M - \tilde{M}\| \leq \varepsilon, \quad \varepsilon \in \mathbb{R}_{\geq 0},$$

where the unknown approximant $\tilde{M} \in \mathbb{R}^{\mathcal{I}}$ fulfils certain rank bounds that will be introduced later. In particular we allow $\varepsilon = 0$ so that the task is to reconstruct the whole tensor $M = \tilde{M}$ in the low rank format. This particular case is considered, e.g. in [11, 3].

1.1. Completion versus Sampling. A tensor fitting problem might arise as follows: the entries $(M_i)_{i \in P}$ could be measurements of a multiparameter model such that each index $i \in P$ represents a specific choice of d parameters. If the measurements are incomplete or in parts known to be incorrect, then the goal is to reconstruct all values of M for all parameter combinations $i \in \mathcal{I}$ from the known values $(M_i)_{i \in P}$ (prior to the assumption that M allows for an approximation in the low rank format). It is crucial that the points P

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are given and we are not free to choose them. In case that the points can be chosen freely one after another, the problem simplifies drastically and can be approached as in [15, 2] by an adaptive sampling strategy. Sometimes one can propose rules on how the entries from P should be chosen, as it is done in quasi Monte Carlo methods. This approach is pursued in [7] and defines sampling rules that allow an efficient approximation scheme. Again, this is different and possibly a simpler task than the tensor completion considered here.

1.2. Low Rank Tensor Formats. The class of tensors in which we aim for a completion of the given tensor entries is a low rank format. In the case $d = 2$ the rank of a tensor coincides with the usual matrix rank, but in dimension $d > 2$ there are several possibilities to define the rank of a tensor and thus there are several data-sparse low rank formats available.

In the $\text{CP}(k)^1$ format or representation

$$A = \sum_{\ell=1}^k \bigotimes_{\mu=1}^d g_{\mu,\ell}, \quad A_{i_1,\dots,i_d} = \sum_{\ell=1}^k \prod_{\mu=1}^d g_{\mu,\ell}(i_\mu), \quad g_{\mu,\ell}(i_\mu) \in \mathbb{R}$$

the tensor completion has been considered in [19, 1, 10]. The minimal number of summands k by which the tensor A can be represented is the *tensor rank* of A , but minimality of k is often not relevant. The $\text{CP}(k)$ format is data sparse in the sense that storing the factors $g_{\mu,\ell}$ amounts to $\mathcal{O}(dnk)$ units (real numbers) of storage, as opposed to the n^d units of the full dense and unstructured tensor A . This is the reason for the attractiveness of the format despite many theoretical and practical difficulties [8].

In the Tucker format

$$A_{i_1,\dots,i_d} = \sum_{\ell_1=1}^{k_1} \cdots \sum_{\ell_d=1}^{k_d} C_{\ell_1,\dots,\ell_d} \prod_{\mu=1}^d g_{\mu,\ell_\mu}(i_\mu), \quad g_{\mu,\ell}(i_\mu) \in \mathbb{R}, \quad C \in \mathbb{R}^{k_1 \times \cdots \times k_d},$$

tensor completion has been considered in [17, 9, 12, 16]. This format is limited to small dimensions d since the so-called core tensor C requires $\prod_{\mu=1}^d k_\mu$ units of storage. The advantage on the other hand is that standard matrix approximation techniques can be used by matricizing the tensor.

The low rank format that we consider lies in between these two, combining the benefits of both: the number of degrees of freedom scales linearly with the dimension d and the format is based on matricizations such that standard linear algebra tools are applicable.

Here, we put no special assumptions on the data points P , except that they are reasonably distributed:

DEFINITION 1.1 (Slices and slice density). *We define the density c_{ov} (or oversampling factor) of a point set $\{M_i \in \mathbb{R} \mid i \in P\}$, $P \subset \mathcal{I}$, in direction $\mu \in D$ and index $\mathbf{j}_\mu \in \mathcal{I}_\mu$ by*

$$c_{ov}(\mathbf{j}_\mu) := \#\{i \in P \mid i_\mu = \mathbf{j}_\mu\}$$

The corresponding slice of a tensor $A \in \mathbb{R}^{\mathcal{I}}$ is defined by

$$A_{i_\mu=\mathbf{j}_\mu} := \hat{A} \in \mathbb{R}^{\mathcal{I}_1 \times \cdots \times \mathcal{I}_{\mu-1} \times \mathcal{I}_{\mu+1} \times \cdots \times \mathcal{I}_d}, \quad \hat{A}_{i_1,\dots,i_{\mu-1},i_{\mu+1},\dots,i_d} := A_{i_1,\dots,i_{\mu-1},\mathbf{j}_\mu,i_{\mu+1},\dots,i_d}$$

Depending on the rank parameters of A (which in turn depend on the target accuracy of the approximation) the slice densities of the set P have to be high enough, i.e.

$$c_{ov}(\mathbf{j}_\mu) > C_{ov}, \quad \mathbf{j}_\mu \in \mathcal{I}_\mu, \quad \mu \in D.$$

¹CP stands for canonical polyadic, in the literature also called CANDECOMP and PARAFAC

If one of the values $c_{ov}(\mathbf{j}_\mu)$ were zero, then this simply means that the slice $A_{i_\mu=j_\mu}$ is undetermined and not observable for any of the low rank formats mentioned above and in the following.

The low rank format under consideration is the hierarchical [5, 4] or TT [14, 13] or MPS [22, 20] format.

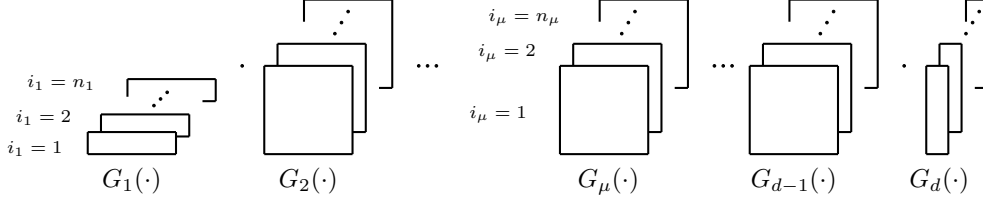


FIG. 1.1. The TT representation of a tensor in $TT(r_1, \dots, r_{d-1})$ with $G_\mu(i_\mu) \in \mathbb{R}^{r_{\mu-1} \times r_\mu}$.

DEFINITION 1.2 (TT tensor format). Let $r_0, \dots, r_d \in \mathbb{N}$ and $r_0 = r_d = 1$. A tensor $A \in \mathbb{R}^{\mathcal{I}}$ of the form or representation

$$A_{i_1, \dots, i_d} = G_1(i_1) \cdots G_d(i_d), \quad G_\mu(i_\mu) \in \mathbb{R}^{r_{\mu-1} \times r_\mu} \quad (1.1)$$

for all $i \in \mathcal{I}$ and $G_\mu : \mathcal{I}_\mu \rightarrow \mathbb{R}^{r_{\mu-1} \times r_\mu}$ is said to be of MPS (matrix product states) format or TT (tensor train) format or hierarchical format, cf. Figure 1.1. We define the set of tensors in TT format by

$$TT(r_1, \dots, r_{d-1}) := \{A \in \mathbb{R}^{\mathcal{I}} \mid A \text{ is of the form (1.1)}\}.$$

The parameters r_μ are called representation ranks and combined to the rank vector $\mathbf{r} := (r_1, \dots, r_{d-1})$. For the matrix blocks $(G_\mu)_{\mu=1}^d$ we use the short notation G . G is called a representation system of A , and if we want to indicate that A is represented by G we write A^G . The minimal ranks r_μ for the representation of a tensor A in TT format are the ranks of certain matricizations of A [4, 15].

The number of degrees of freedom or parameters in the MPS representation is in

$$\mathcal{O} \left(\sum_{\mu=1}^d r_{\mu-1} r_\mu n_\mu \right) \sim \mathcal{O}(dr^2n), \quad r := \max_{\mu \in D} r_\mu, \quad n := \max_{\mu \in D} n_\mu.$$

It could thus in principle be possible to reconstruct the tensor from a number of samples that is in $\mathcal{O}(\log N)$ for a tensor having $N = \prod_{i=1}^d n_i$ entries, cf. Section 4.3.

1.3. Statement of the Main Approximation Problem. The full approximation problem can be stated as follows. For $S \subset \mathcal{I}$ let

$$\|X\|_F := \sqrt{\sum_{i \in \mathcal{I}} X_i^2}, \quad (X|_S)_i := \begin{cases} X_i & \text{if } i \in S \\ 0 & \text{otherwise} \end{cases}, \quad \|X\|_S := \|X|_S\|_F.$$

PROBLEM 1.3 (Main problem). Given a tensor $M \in \mathbb{R}^{\mathcal{I}}$ known only at points $P \subset \mathcal{I}$, and given representation ranks r_1, \dots, r_{d-1} , find a representation (1.1) with representation system G such that $A = A^G$ fulfils

$$A = \operatorname{argmin}_{\tilde{A} \in TT(r_1, \dots, r_{d-1})} \|M - \tilde{A}\|_P.$$

A related approach for tensor completion is presented in [18] where the authors use a steepest descent iteration on the tensor manifold. Our approach, the alternating directions fitting (ADF) algorithm, is based on ideas from LMaFit for matrix completion [21]; and we generalize these to tensor completion.

1.4. First Order Optimality. For a representation system $(G_\mu)_{\mu=1}^d$ such that $A = A^G$ one can write the main problem in the form

$$G = \underset{\tilde{G}}{\operatorname{argmin}} \|M - A^{\tilde{G}}\|_P$$

and by introducing an additional tensor $Z \in \mathbb{R}^{\mathcal{I}}$, G can be found via the task to

$$\operatorname{minimize} f(G, Z) := \|Z - A^G\|_F \quad \text{s.t.} \quad Z|_P = M|_P, \quad A^G \in TT(r_1, \dots, r_{d-1}).$$

The latter function f yields first order optimality conditions

$$Z|_{\mathcal{I} \setminus P} = A^G|_{\mathcal{I} \setminus P} \quad \text{and} \quad G_\mu = \underset{G_\mu}{\operatorname{argmin}} \|Z - A^G\|_P.$$

Solving this nonlinear system of equations simultaneously for G_1, \dots, G_d, Z is not trivial. In a hard or soft thresholding iteration one would have to find a best approximation A^G to a given tensor Z , and in the matrix case $d = 2$ this is expensive but possible. For tensors in $d > 2$ such a best approximation is not available. A common technique for finding something close to a best approximation is an alternating fit cycling through the unknowns G_μ . But since our final goal is not the approximation of Z but the minimization of f , it makes sense to directly solve the nonlinear system by an alternating fit. We approach this nonlinear system by a nonlinear block Gauß-Seidel iteration where the blocks of unknowns are G_1, \dots, G_d, Z :

Require: Initial guess A^G

for $i=1, \dots$ **do**

For all $i \in \mathcal{I} \setminus P$ set $Z_i := A_i^G$ and for all $i \in P$ set $Z_i := M_i$

For all $\mu \in D$ minimize $\|Z - A^G\|_F$ with respect to G_μ

end for

Finally, we use (partial) successive overrelaxation in order to speed up the convergence, and we change the order of optimization of blocks to be $Z, G_1, \dots, G_h, Z, G_d, \dots, G_h$ for some fixed $h \in D$. Altogether this defines the basic proceeding of the alternating directions fit (ADF) Algorithm 1 by which we solve the tensor completion problem.

1.5. Organization of the Article. In Section 2 we introduce the necessary basic tools for the analysis and algorithmic treatment of the tensor approximation problem. Section 3 presents the ADF algorithm in detail and analyses the computational and storage complexity of one iterative step. Several practical issues like adaptive choice of the ranks, improved performance, and stopping criteria are considered. In the numerical examples Section 4 we apply our algorithm to two classes of examples: a) smooth function related tensors, and b) random low rank tensors with and without noise. We end with a conclusion in Section 5.

2. Optimization in TT-Format.

2.1. Matrix Fitting. We first present a central tool, by which a k -rank approximation of a sparsely known matrix can be obtained quite efficiently, cf. [21].

Algorithm 1 Basic proceeding of the ADF algorithm

Require: Initial guess A^G , overrelaxation parameter $\alpha \geq 1$

while breaking condition not fulfilled **do**

For all $i \in \mathcal{I} \setminus P$ set $Z_i := A_i^G$ and for all $i \in P$ set $Z_i := M_i$

for $\mu = 1, \dots, h$ **do**

Determine $G_\mu^+ := \operatorname{argmin}_{G_\mu} \|Z - A^G\|_F$ and set $G_\mu := G_\mu + \alpha(G_\mu^+ - G_\mu)$

end for

For all $i \in \mathcal{I} \setminus P$ set $Z_i := A_i^G$ and for all $i \in P$ set $Z_i := M_i$

for $\mu = d, \dots, h$ **do**

Determine $G_\mu^+ := \operatorname{argmin}_{G_\mu} \|Z - A^G\|_F$ and set $G_\mu := G_\mu + \alpha(G_\mu^+ - G_\mu)$

end for

end while

THEOREM 2.1 (LMaFit principle). *Let $W \in \mathbb{R}^{n \times m}$ and $Y \in \mathbb{R}^{k \times m}$ be given matrices and Y of full rank k . Define $X \in \mathbb{R}^{n \times k}$ as the minimizer*

$$X := \operatorname{argmin}_{\tilde{X}} \|W - \tilde{X}Y\|_F$$

Then we gain

$$\operatorname{range}(WY^T) = \operatorname{range}(X).$$

Proof. ([21]) Using the SVD of $Y = U\Sigma V^T$ we have the pseudo inverse $Y^+ = V\Sigma^+U^T$. Hence $X = WV\Sigma^+U^T$, while $WY^T = WV\Sigma U^T$. Thereby $\operatorname{range}(WY^T) = \operatorname{range}(X)$. \square

Fortunately, the LMaFit principle also proves to be a very useful tool in the approximation of a sparsely known tensor of TT-ranks r_1, \dots, r_{d-1} with the help of the representation G . It takes, however, some preparation until its use can be justified.

2.2. Statement of the Lefthand and Righthand Approximation Problem.

For practical reasons (based on the LMaFit principle) it is most efficient if in Algorithm 1 the blocks G_1, \dots, G_h or G_d, \dots, G_h are optimized consecutively, where the direction h can be anything between 1 and d . Since we would like to update Z not only after all blocks G_μ are optimized but earlier, we choose

$$h := \lfloor (d+1)/2 \rfloor. \quad (2.1)$$

PROBLEM 2.2 (Lefthand problem). *Given a tensor $Z \in \mathbb{R}^{\mathcal{I}}$ (all entries known), ranks \mathbf{r} , and a starting representation G , replace for $\mu = 1, \dots, h$ the entries of G_μ such that $G_\mu = \operatorname{argmin}_{G_\mu} \|Z - A^G\|_F$. In order to avoid confusion we want to remark that the task for the lefthand problem is neither to find the minimizer (G_1, \dots, G_d) nor the partial minimizer (G_1, \dots, G_h) . Instead, we seek consecutively the partial minimizers in the stated order*

$$G_1 := \operatorname{argmin}_{G_1} \|Z - A^G\|_F, G_2 := \operatorname{argmin}_{G_2} \|Z - A^G\|_F, \dots, G_h := \operatorname{argmin}_{G_h} \|Z - A^G\|_F.$$

PROBLEM 2.3 (Righthand problem). *Given a tensor $Z \in \mathbb{R}^{\mathcal{I}}$ (known at all points), ranks \mathbf{r} , and a starting representation G , replace for $\mu = d, \dots, h$ the entries of G_μ such that $G_\mu = \operatorname{argmin}_{G_\mu} \|Z - A^G\|_F$.*

2.3. Tensor Calculus. In this section we introduce the necessary tools to work with matrix blocks in order to construct and prove the core step of the ADF algorithm (Theorem 3.1).

DEFINITION 2.4 (Matrix block). *Let $k_1, k_2, n \in \mathbb{N}$. We define a matrix block $H \in (\mathbb{R}^{k_1 \times k_2})^n$ as a vector of matrices $H(1), \dots, H(n) \in \mathbb{R}^{k_1 \times k_2}$. We call $k_1 \times k_2$ the dimension and n the length of H .*

REMARK 2.5 (Algebraic properties). *Let $k_1, k_2 \in \mathbb{N}$ be fixed. Then the set of matrix blocks $H \in (\mathbb{R}^{k_1 \times k_2})^n$ forms an \mathbb{R} -vectorspace. Additionally, it can also be viewed as left-module over the non-abelian matrix ring $\mathbb{R}^{k_1 \times k_1}$ as well as right-module over $\mathbb{R}^{k_2 \times k_2}$. Next we introduce a tool to combine multiple matrix blocks into one, which is ultimately used for the definition of the TT representation A^G .*

DEFINITION 2.6 ((Kronecker) product between matrix blocks). *We define the (Kronecker) product \otimes for matrix blocks H_1, H_2 of dimensions $k_1 \times k_m, k_m \times k_2$ and lengths n_1, n_2 as*

$$(H_1 \otimes H_2)((i, j)) := H_1(i)H_2(j)$$

where $(H_1 \otimes H_2)$ is a matrix block of dimension $k_1 \times k_2$ and length $n_1 n_2$. Note that this is analogous to the conventional Kronecker product, but $(H_1 \otimes H_2)^T$ does neither equal $H_1^T \otimes H_2^T$ nor $H_2^T \otimes H_1^T$. In order to simplify the notation we use the following convention:

- We treat the product of a matrix and a matrix block as if the matrix was a block of length 1 and skip the \otimes . It is referred to as pointwise multiplication.
- We write $(H_1 \otimes \dots \otimes H_n)(i_1 \dots i_n)$ instead of $(H_1 \otimes \dots \otimes H_n)((i_1 \dots i_n))$.
- The empty Kronecker product is defined to be I , the identity matrix of suitable size.

REMARK 2.7 (Generating A^G). *Using the Kronecker product, one can express A^G by*

$$A_{(i_1, \dots, i_d)}^G = (G_1 \otimes \dots \otimes G_d)(i_1, \dots, i_d), \quad A^G = G_1 \otimes \dots \otimes G_d.$$

Next, we define operations to switch between matrix blocks, matrices, and tensors.

DEFINITION 2.8 (Lefthand block and righthand block). *Let $H \in (\mathbb{R}^{k_1 \times k_2})^n$ be a matrix block. We define the lefthand block $H]$ as*

$$H] := \begin{bmatrix} H(1) \\ H(2) \\ \vdots \\ H(n) \end{bmatrix} \in \mathbb{R}^{n k_1 \times k_2}, \quad \begin{array}{c} \boxed{\vdots} \\ \boxed{\vdots} \\ \boxed{\vdots} \end{array} \xrightarrow{\cdot] } \begin{array}{|c|} \hline \vdots \\ \hline \vdots \\ \hline \end{array} \quad (2.2)$$

and the righthand block $[H$ as

$$[H := [H(1) \ H(2) \ \dots \ H(n)] \in \mathbb{R}^{k_1 \times n k_2}, \quad \begin{array}{c} \boxed{\vdots} \\ \boxed{\vdots} \\ \boxed{\vdots} \end{array} \xrightarrow{[\cdot} \begin{array}{|c|c|c|} \hline \vdots & \dots & \vdots \\ \hline \end{array} \quad (2.3)$$

The transpose H^T of a matrix block is defined as $H^T(i) := H(i)^T$.

REMARK 2.9 (Conjugacy of block operations). *The lefthand block operation is conjugate to the righthand block operation by means of*

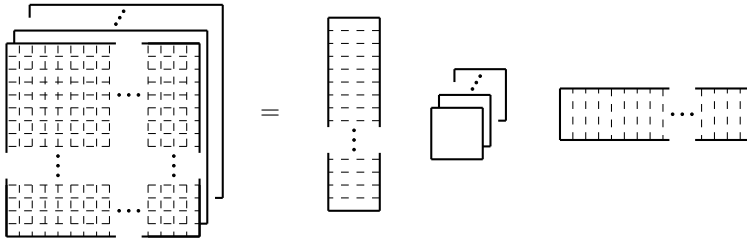
$$(\cdot)^T \circ \cdot] = [\cdot \circ (\cdot)^T.$$

DEFINITION 2.10 (Block matricization). Let $A \in \mathbb{R}^{\mathcal{I}}$ be a d -dimensional tensor. A block matricization with respect to $s \in \{1, \dots, d\}$, $A_{(s)}$, is defined as the matrix block of dimension $(n_1 \dots n_{s-1}) \times (n_{s+1} \dots n_d)$ and length n_s , given by

$$(A_{(s)}(i_s))_{(i_1, \dots, i_{s-1}), (i_{s+1}, \dots, i_d)} := A_{i_1, \dots, i_d}, \quad \forall i_s \in \mathcal{I}_s.$$

EXAMPLE 2.11 (Block matricization of A^G). For a better understanding one may have a look at the following equation, which is valid for any s and representation G :

$$A_{(s)}^G = (G_1 \otimes \dots \otimes G_{s-1}) \lceil G_s \rceil [(G_{s+1} \otimes \dots \otimes G_d)].$$



Note that both the multiplication with the lefthand as well as righthand block is elementwise, i.e. $A_{(s)}(i_s)_{(i_1, \dots, i_{s-1}), (i_{s+1}, \dots, i_d)} = (G_1(i_1) \dots G_{s-1}(i_{s-1})) G_s(i_s) (G_{s+1}(i_{s+1}) \dots G_d(i_d))$.

For further calculations we give a scalar product for matrix blocks and derive a norm, which is essentially the Frobenius norm.

DEFINITION 2.12 ((Scalar) product of matrix blocks). Let G and H be matrix blocks of the dimensions $k_1 \times k_m, k_m \times k_2$ and same length. Then we define the (scalar) product of two matrix blocks as

$$\langle G, H \rangle := \sum_i G(i)H(i) = \lceil GH \rceil \in \mathbb{R}^{k_1 \times k_2}.$$

For a matrix $J \in \mathbb{R}^{k_m \times k_m}$ we define

$$\langle G, J, H \rangle := \langle GJ, H \rangle = \langle G, JH \rangle.$$

Note that $\langle \cdot, \cdot \rangle$ is only a product with scalar output regarding its module properties.

DEFINITION 2.13 (\mathbb{R} -scalar product and matrix block norm). Let $V := (\mathbb{R}^{k_1 \times k_2})^n$ be the \mathbb{R} -Vectorspace of matrix blocks of dimension $k_1 \times k_2$ and length n . Then $\langle \cdot, \cdot \rangle$ defines a scalar product $\langle \cdot, \cdot \rangle_{\mathbb{R}}$ on V via

$$\langle G, H \rangle_{\mathbb{R}} := \text{trace} \langle G, H^T \rangle = \text{trace} \langle G^T, H \rangle, \quad G, H \in V.$$

The corresponding norm $\|\cdot\|$ on V is defined as $\|G\| := \sqrt{\langle G, G \rangle_{\mathbb{R}}}$.

REMARK 2.14 (Properties of the matrix block norm). For a matrix block G , tensor A and index $s \in D$ holds

$$\|G\| = \sqrt{\sum_i \|G(i)\|_F^2}, \quad \|A\|_F = \|A_{(s)}\|.$$

We introduce the concept of orthogonality (cf. [6]) for matrix blocks, by which we can greatly simplify the minimization problem.

DEFINITION 2.15 (Orthogonality of matrix blocks). For a matrix block H , we call H lefthand orthogonal if the columns of H are orthogonal (this being $\langle H^T, H \rangle = I$), and

riighthand orthogonal if the rows of $\lceil H$ are orthogonal (this being $\langle H, H^T \rangle = I$).

Let Q be a matrix block of same dimensions as H . We then define the (non-unique) operation orth^ℓ such that for $Q = \text{orth}^\ell(H)$, the pair $(Q \lceil, R)$ is a QR-decomposition of $H \lceil$. Then Q is lefthand orthogonal and $QR = H$.

Likewise orth^r is such that for $Q = \text{orth}^r(H)$, the pair $(L, \lceil Q)$ is an LQ-decomposition of $\lceil H$. Then Q is righthand orthogonal and $LQ = H$. In the following we demonstrate how orthogonality, the scalar product and the Kronecker product act together and form a central result (Corollary 2.18) regarding the feasibility (Theorem 3.4) of the ADF core step (Theorem 3.1) for which we initially only need Corollary 2.17.

LEMMA 2.16 (Scalar products of Kronecker products). *Let G_1, G_2 and H_1, H_2 be matrix blocks of appropriate dimensions and lengths. Then*

$$\langle (G_1 \otimes G_2)^T, H_1 \otimes H_2 \rangle = \langle G_2^T, \langle G_1^T, H_1 \rangle, H_2 \rangle,$$

respectively

$$\langle G_1 \otimes G_2, (H_1 \otimes H_2)^T \rangle = \langle G_1, \langle G_2, H_2^T \rangle, H_1^T \rangle.$$

Proof. Due to analogy we consider only the first case. By definition and reordering of summation we get

$$\begin{aligned} \langle (G_1 \otimes G_2)^T, H_1 \otimes H_2 \rangle &= \sum_i ((G_1 \otimes G_2)(i))^T (H_1 \otimes H_2)(i) \\ &= \sum_{i_1, i_2} G_2(i_2)^T G_1(i_1)^T (H_1(i_1) H_2(i_2)) = \sum_{i_2} G_2(i_2)^T \sum_{i_1} (G_1(i_1)^T H_1(i_1)) H_2(i_2) \\ &= \sum_{i_2} G_2(i_2)^T \langle G_1^T, H_1 \rangle H_2(i_2) = \langle G_2^T, \langle G_1^T, H_1 \rangle, H_2 \rangle. \end{aligned}$$

□

COROLLARY 2.17 (Orthogonality of Kronecker products). *If two matrix blocks G, H are lefthand (riighthand) orthogonal, then $G \otimes H$ is lefthand (riighthand) orthogonal. This follows as for a matrix block K and a lefthand (riighthand) orthogonal matrix block Q (P), we have*

$$\langle (Q \otimes K)^T, Q \otimes K \rangle = \langle K^T, K \rangle \quad \text{and} \quad \langle K, K^T \rangle = \langle K \otimes P, (K \otimes P)^T \rangle, \text{ respectively.}$$

Furthermore this implies

$$\|Q \otimes K\| = \|K\| = \|K \otimes P\|.$$

COROLLARY 2.18 (Scalar products of multiple Kronecker products). *Let G_1, \dots, G_ℓ and H_1, \dots, H_ℓ be matrix blocks of appropriate dimensions. Let $G := G_1 \otimes \dots \otimes G_\ell$ and $H := H_1 \otimes \dots \otimes H_\ell$. Then*

$$\langle G^T, H \rangle = \langle G_\ell^T, \dots, \langle G_1^T, H_1 \rangle, \dots, H_\ell \rangle.$$

If $G_1 = H_1, \dots, G_k = H_k$ are lefthand orthogonal, we have

$$\langle G^T, H \rangle = \langle G_\ell^T, \dots, \langle G_{k+1}^T, H_{k+1} \rangle, \dots, H_\ell \rangle = \langle (G_{k+1} \otimes \dots \otimes G_\ell)^T, H_{k+1} \otimes \dots \otimes H_\ell \rangle.$$

Likewise

$$\langle G, H^T \rangle = \langle G_1, \dots, \langle G_\ell, H_\ell^T \rangle, \dots, H_1^T \rangle.$$

If $G_k = H_k, \dots, G_\ell = H_\ell$ are righthand orthogonal, we have

$$\langle G, H^T \rangle = \langle G_1, \dots, \langle G_{k-1}, H_{k-1}^T \rangle, \dots, H_1^T \rangle = \langle G_1 \otimes \dots \otimes G_{k-1}, (H_1 \otimes \dots \otimes H_{k-1})^T \rangle.$$

Note that this decouples the Kronecker product and reduces the amount of computations as well as the involved dimensions. For shorter notation we set the empty scalar product (i.e. $\ell = 0$) as I , the identity matrix of suitable size. We offer a last remark on a property which is central to the ADF core step.

REMARK 2.19 (Non-uniqueness of representations). Considering $A^{(\cdot)} : H \mapsto A^H$, one has a mapping which is non-injective as for the representations $H^1 : H_1, \dots, (H_\ell J), \dots, H_d$ and $H^2 : H_1, \dots, (JH_{\ell+1}), \dots, H_d$ one has $A^{H^1} = A^{H^2}$, where ℓ is arbitrary and J a square matrix of appropriate dimension. This degree of freedom is not a disadvantage, indeed we exploit this property in Theorem 3.1 by use of the LMaFit principle (Theorem 2.1). Furthermore one can always assume, using the operations orth^ℓ and orth^r , that all matrix blocks H_i , $i < h$ are lefthand orthogonal as well as that all matrix blocks H_i , $i > h$ are righthand orthogonal. Then also $\|A^G\|_F = \|G_h\|$.

3. The ADF Algorithm. We approach the main Problem 1.3 by the ADF Algorithm 1. As a basic step of the algorithm one has to solve the lefthand and righthand problem, i.e., optimize with respect to G_1, \dots, G_h or G_d, \dots, G_h while keeping the other variables fixed. In the following we give a detailed description for solving these problems, as well as for the choice of the overrelaxation parameter α (Remark 3.8 and Algorithm 2).

3.1. The ADF Core Step. The core step we now give solves the lefthand respectively righthand problem in the sense that G_1, \dots, G_h , respectively G_d, \dots, G_h , are each optimized individually as it is required for the update of G in Algorithm 1.

THEOREM 3.1 (Core step of the ADF algorithm). Given the lefthand problem one can, as one sequence, optimize consecutively G_1, \dots, G_h in order $s = 1 \rightarrow h$, respectively G_h, \dots, G_d in order $s = h \leftarrow d$ when given the righthand problem. Without loss of generality we assume that $G_1 \dots G_{h-1}$ are given lefthand orthogonal, respectively $G_{h+1} \dots G_d$ righthand orthogonal (cf. Remark 2.19). The solution of the lefthand or righthand problem is given by

$$G_s(\mathbf{j}) = \sum_{i \in \mathcal{I}, i_s = \mathbf{j}} Z_i(G_1(i_1) \dots G_{s-1}(i_{s-1}))^T (G_{s+1}(i_{s+1}) \dots G_d(i_d))^T = Q_s^T Z_{(s)}(\mathbf{j}) P_s^T$$

where

$$Q_s := (G_1 \otimes \dots \otimes G_{s-1}), \quad P_s := [(G_{s+1} \otimes \dots \otimes G_d),$$

followed by

$$G_s \leftarrow \begin{cases} \text{orth}^\ell(G_s), & \text{if } s < h \\ G_s, & \text{if } s = h \\ \text{orth}^r(G_s), & \text{if } s > h. \end{cases}$$

Proof. (lefthand) We carry out the proof for $s < h$ and $s = h$, assuming that the steps before were performed as described above. Thereby $G_1 \dots G_{s-1}$ are lefthand orthogonal.

We abbreviate $P := P_s$ and $Q := Q_s$. As Q is orthogonal we have

$$\begin{aligned} G_s &= \operatorname{argmin}_{G_s} \|Z - A^G\|_F = \operatorname{argmin}_{G_s} \|Z_{(s)} - A_{(s)}^G\| = \operatorname{argmin}_{G_s} \|Z_{(s)} - QG_sP\| \\ &= \operatorname{argmin}_{G_s} \|Q^T Z_{(s)} - G_sP\| = \operatorname{argmin}_{G_s} \|(Q^T Z_{(s)})] - G_s]P\|_F \quad (LS), \end{aligned}$$

the latter being one single least squares problem to be solved for the matrix $G_s]$.

Case $s < h$: At this point we can, for $s < h$, use the LMaFit principle. We thereby know that

$$\operatorname{range}((Q^T Z_{(s)})]P^T) = \operatorname{range}(G_s]),$$

which for some matrix R yields

$$(Q^T Z_{(s)})]P^T R = G_s] \Leftrightarrow Q^T Z_{(s)}(i_s)P^T R = G_s(i_s) \quad \forall i_s.$$

In principle we have found G_s , but we do certainly not want to calculate R . Therefore, we interpret R as part of G_{s+1} instead of G_s . This is a valid operation that does not change A^G , as

$$\begin{aligned} &\dots G_{s-1}(i_{s-1}) (Q^T Z_{(s)}(i_s)P^T \mathbf{R}) G_{s+1}(i_{s+1}) \dots \\ &= \dots G_{s-1}(i_{s-1}) (Q^T Z_{(s)}(i_s)P^T) (\mathbf{R}G_{s+1}(i_{s+1})) \dots \quad \forall (i_1, \dots, i_d) \in \mathcal{I}. \end{aligned}$$

Thereby R will vanish as the newly formed $\mathbf{R}G_{s+1}$ is next to be replaced. Hence we can, instead of the direct minimizer, choose

$$G_s(i_s) \leftarrow Q^T Z_{(s)}(i_s)P^T \quad \forall i_s. \quad (*)$$

followed by lefthand orthogonalizing G_s . This again produces some R , which is treated likewise (cf. [6] for the matrix case).

Case $s = h$: One can see a more specific reason for the splitting into lefthand and righthand now. There is naturally a limit for R to be transferred to the right, at the latest G_d . This implies that we can neither use the LMaFit principle nor orthogonalize for one index, this being $s = h$. Yet in this case P is orthogonal. Starting at (LS) again, we can thereby without any further reasoning put P to the right as we did with Q . This immediately results in the same formula (*), except that we do not orthogonalize. This completes the proof. \square

The core step described above solves the lefthand (or righthand) problem without overrelaxation. The overrelaxation parameter α can be incorporated directly into the core step by modifying Z as follows.

LEMMA 3.2. *Let $A^G = G_1 \otimes \dots \otimes G_d \in \mathbb{R}^{\mathcal{I}}$ be given, $\alpha \in \mathbb{R}$, $Z \in \mathbb{R}^{\mathcal{I}}$ and*

$$G_\mu^+ := \operatorname{argmin}_{\tilde{G}_\mu} \|Z - G_1 \otimes \dots \otimes G_{\mu-1} \otimes \tilde{G}_\mu \otimes G_{\mu+1} \otimes \dots \otimes G_d\|.$$

Then $G_\mu^\alpha := \alpha G_\mu^+ + (1 - \alpha)G_\mu$ fulfils

$$G_\mu^\alpha = \operatorname{argmin}_{\tilde{G}_\mu} \|Z^\alpha - G_1 \otimes \dots \otimes G_{\mu-1} \otimes \tilde{G}_\mu \otimes G_{\mu+1} \otimes \dots \otimes G_d\|$$

for $Z^\alpha := \alpha Z + (1 - \alpha)A^G$.

Proof. We insert $\alpha G_\mu^+ + (1 - \alpha)G_\mu$ into the righthand side of the last equation and obtain

$$\begin{aligned}
& \|Z^\alpha - G_1 \otimes \cdots \otimes G_{\mu-1} \otimes (\alpha G_\mu^+ + (1 - \alpha)G_\mu) \otimes G_{\mu+1} \otimes \cdots \otimes G_d\| \\
&= \|\alpha Z + (1 - \alpha)A^G - G_1 \otimes \cdots \otimes G_{\mu-1} \otimes (\alpha G_\mu^+ + (1 - \alpha)G_\mu) \otimes G_{\mu+1} \otimes \cdots \otimes G_d\| \\
&= \|\alpha Z - \alpha G_1 \otimes \cdots \otimes G_{\mu-1} \otimes G_\mu^+ \otimes G_{\mu+1} \otimes \cdots \otimes G_d\| \\
&= \alpha \|Z - G_1 \otimes \cdots \otimes G_{\mu-1} \otimes G_\mu^+ \otimes G_{\mu+1} \otimes \cdots \otimes G_d\|
\end{aligned}$$

and any other choice $\tilde{G}_\mu = \alpha \tilde{G}_\mu^+ + (1 - \alpha)G_\mu$ does not give a smaller value since G_μ^+ is a minimizer. \square

NOTATION 3.3 (Denoting current and old representations). *During one sweep of updating G_1, \dots, G_h in the lefthand problem, we use the notation G^- for the representation before the sweep and G for the updated representation. Analogously for the righthand problem.*

THEOREM 3.4 (Practical ADF core step (lefthand)). *Under the assumptions from Theorem 3.1 the update G_1, \dots, G_h for the lefthand problem with overrelaxation parameter α is given by*

$$G_s(\mathbf{j}) = \underbrace{\langle G_{s-1}^T, \dots, \langle G_1^T, G_1^- \rangle \dots G_{s-1}^- \rangle}_{(LS_s^1)} G_s^-(\mathbf{j}) \underbrace{\langle G_{s+1}^- \dots \langle G_h^-, G_h^{-T} \rangle \dots G_{s+1}^{-T} \rangle}_{(LS_s^2)} \quad (3.1)$$

$$+ \sum_{\substack{i=(i_1, \dots, i_d) \in P \\ i_s = \mathbf{j}}} \alpha (M_i - A_i^{G^-}) \underbrace{(G_1(i_1) \dots G_{s-1}(i_{s-1}))^T}_{(LM_s^1)_i} \underbrace{(G_{s+1}^-(i_{s+1}) \dots G_d^-(i_d))^T}_{(LM_s^2)_i} \quad (3.2)$$

$$G_s \leftarrow \begin{cases} \text{orth}^\ell(G_s), & \text{if } s < h \\ G_s, & \text{if } s = h. \end{cases} \quad (3.3)$$

(The short notations are used for Lemma 3.5.)

Proof. According to Theorem 3.1 and Lemma 3.2, we have

$$\begin{aligned}
G_s(\mathbf{j}) &= Q_s^T Z_{(s)}^\alpha(\mathbf{j}) P_s^T \\
&= \sum_{\substack{i=(i_1, \dots, i_d) \in \mathcal{I} \\ i_s = \mathbf{j}}} Z_i^\alpha (G_1(i_1) \dots G_{s-1}(i_{s-1}))^T (G_{s+1}(i_{s+1}) \dots G_d(i_d))^T \quad \forall \mathbf{j}. \quad (3.4)
\end{aligned}$$

$Z = A^{G^-}|_{\mathcal{I} \setminus P} + M|_P$ (cf. Algorithm 1) and $Z^\alpha = \alpha Z + (1 - \alpha)A^{G^-}$ (cf. Lemma 3.2) yield

$$Z^\alpha = \underbrace{A^{G^-}}_{\leftrightarrow \text{First summand}} + \alpha \underbrace{(M|_P - A^{G^-}|_P)}_{\leftrightarrow \text{Second summand}}$$

which we insert it into (3.4).

First summand: Recall that $A_{(s)}^{G^-}$ can be expanded (Example 2.11). Using the definition for Q_s and P_s (Theorem 3.1) we have:

$$\begin{aligned}
& Q_s^T A_{(s)}^{G^-}(\mathbf{j}) P_s^T = \\
& (G_1 \otimes \cdots \otimes G_{s-1})^T (G_1^- \otimes \cdots \otimes G_{s-1}^-) G_s^-(\mathbf{j}) [(G_{s+1}^- \otimes \cdots \otimes G_d^-) (G_{s+1} \otimes \cdots \otimes G_d)^T \quad (3.5)
\end{aligned}$$

With Remark 2.9 and the definition for the scalar product (Definition 2.12) we can simplify

$$(3.5) = \langle (G_1 \otimes \dots \otimes G_{s-1})^T, (G_1^- \otimes \dots \otimes G_{s-1}^-) \rangle G_s^-(i_s) \langle (G_{s+1}^- \otimes \dots \otimes G_d^-), (G_{s+1} \otimes \dots \otimes G_d)^T \rangle$$

Due to Corollary 2.18 and the fact that G_{s+1}, \dots, G_d still equal G_{s+1}^-, \dots, G_d^- and are righthand orthogonal as of index $h+1$ when optimizing lefthand we can simplify both scalar products

$$(3.5) = \langle G_{s-1}^T, \dots \langle G_1^T, G_1^- \rangle \dots G_{s-1}^- \rangle G_s^-(j) \langle G_{s+1}^- \dots \langle G_h^-, G_h^{-T} \rangle \dots G_{s+1}^{-T} \rangle.$$

Second summand: As $(M|_P - A^{G^-}|_P)_i = 0$ for any $i \notin P$, we can reduce the summation from \mathcal{I} to P without changing its outcome. We use again that G_{s+1}, \dots, G_d still equal G_{s+1}^-, \dots, G_d^- and receive the formula stated in the theorem. \square

Analogously to the lefthand case we can treat the righthand case by

$$\begin{aligned} G_s(j) &= \langle G_{s-1}^{-T}, \dots \langle G_h^{-T}, G_h^- \rangle \dots G_{s-1}^- \rangle G_s^-(j) \langle G_{s+1}^- \dots \langle G_d^-, G_d^T \rangle \dots G_{s+1}^T \rangle \\ &\quad + \sum_{\substack{i=(i_1, \dots, i_d) \in P \\ i_s=j}} \alpha(M_i - A_i^{G^-}) (G_1^-(i_1) \dots G_{s-1}^-(i_{s-1}))^T (G_{s+1}(i_{s+1}) \dots G_d(i_d))^T \\ G_s &\leftarrow \begin{cases} \text{orth}^T(G_s), & \text{if } s > h \\ G_s, & \text{if } s = h. \end{cases} \end{aligned}$$

3.2. Computational Complexity of ADF. Each statement in this section which we give in its lefthand version can be treated analogously in the righthand case, leading to equivalent results.

LEMMA 3.5 (Successive computing). *In the lefthand core step (Theorem 3.4) occuring terms can be reduced to simpler successive computations, via:*

$$(LS_s^1) = \langle G_{s-1}^T, (LS_{s-1}^1), G_{s-1}^- \rangle, \quad (3.6)$$

$$(LS_s^2) = \langle G_{s+1}^{-T}, (LS_{s+1}^2), G_{s+1}^- \rangle, \quad (3.7)$$

where $(LS_1^1) = 1$ and $(LS_h^2) = I$ (the identity matrix). Likewise

$$(LM_s^1)_i = G_{s-1}(i_{s-1})^T (LM_{s-1}^1)_i, \quad (3.8)$$

$$(LM_s^2)_i = (LM_s^2)_i G_{s+1}^-(i_{s+1})^T \quad (3.9)$$

where $(LM_1^1) = 1$ and (LM_h^2) is inherited from the righthand step. Hence, while (LS^1) and (LM^1) are updated within the sequence, (LS^2) and (LM^2) are calculated before. Furthermore, (LM_h^1) and (LM_h^2) can be used to update $A_P^{G^-}$.

COROLLARY 3.6 (Computational complexity). *Let $r := \max\{r_1, \dots, r_{d-1}\}$, $n := \max\{n_1, \dots, n_d\}$ and $p := \#P$. If we consider one full lefthand optimization sweep (Z, G_1, \dots, G_h) , we can give an upper bound for the effort by analyzing the operations in Lemma 3.5 and Theorem 3.4:*

1. (3.6) \mathcal{E} (3.7): $2n$ times $(r \times r)$ times $(r \times r)$ matrix multiplications
2. (3.8) \mathcal{E} (3.9): p times $(1 \times r)$ times $(r \times r)$ matrix multiplications
3. (3.1): n times $(r \times r)$ times $(r \times r)$ matrix multiplications
4. (3.2): p times $(r \times 1)$ times $(1 \times r)$ matrix multiplications
5. (3.3): at most one QR decomposition of an $nr \times r$ matrix

Each of these steps is performed about $d/2$ times. As the number of samples scales like $p \sim C_{ov}r^2nd$, items 1, 3, 5 are negligible. This leaves us with a total effort for one lefthand sweep of

$$\mathfrak{C} = \mathcal{O}(pr^2d) = \mathcal{O}(C_{ov}r^4nd^2),$$

where the oversampling constant C_{ov} is assumed to be the uniform slice density, cf. Definition 1.1. Note that the constant hidden in the order is very small, but the number of necessary lefthand and righthand sweeps can be large.

COROLLARY 3.7 (Storage complexity). *Let $r := \max\{r_1, \dots, r_{d-1}\}$ and $p := \#P$ and $n := \max\{n_1, \dots, n_d\}$. As in the lefthand case (LS^2) and (LM^2) have to be calculated beforehand and stored for efficiency reasons, we require*

$$\mathfrak{S} = \mathcal{O}(prd) = \mathcal{O}(C_{ov}r^3nd^2)$$

numbers to be stored.

3.3. Choice of the SOR Parameter α . By an optimized determination of the acceleration parameter α one can speed up the convergence of the ADF algorithm considerably. Therefore, after each sweep for the lefthand or righthand problem, we allow a relatively expensive search for a suitable α by testing increased (α^{up}) and reduced (α^{down}) values of α until the residual decays (or we break).

REMARK 3.8 (Determination of the direction). *To handle the acceleration parameter α , we introduce a second parameter δ taking the role of an increment. Each lefthand or righthand sweep is run for two different accelerations ($\alpha^{up}, \alpha^{down}$), where we denote by α the previous one:*

$$\alpha^{up} := \alpha + \delta, \quad \alpha^{down} := \max\{1, \alpha - \delta/5.\}$$

By this choice the overrelaxation parameter is at least $\alpha \geq 1$. Depending on the residuals of the results, one of the three directions, denoted by (up), (down) or (back), is chosen as specified in Algorithm 2. It determines the new α , δ as well as G . At the start we use $\alpha := 1$ (possibly adapted to the problem) and $\delta := \alpha/4$.

Algorithm 2 Choice of the SOR parameter α

Let G^- be the old representation received by having used α . Let G^{up}, G^{down} denote the representation obtained by either a lefthand or righthand sweep with parameter $\alpha^{up}, \alpha^{down}$ leading to residuals R^-, R^{up}, R^{down} .

Notation: \searrow = decrease, $\searrow\searrow$ = heavy decrease, \nearrow = increase

```

if  $R^{up} > R^-$  and  $R^{down} > R^-$  then
   $\searrow\searrow \alpha$  (but  $\alpha \geq 1$ );  $\searrow \delta$ ; keep  $G \leftarrow G^-$  and repeat step;  $\Gamma \leftarrow$  (back);
else if ( $R^{up} < R^{down}$ ) then
  If  $\Gamma =$  (up) then  $\nearrow \delta$ , otherwise  $\searrow \delta$ ;
   $\alpha \leftarrow \alpha^{up}$ ;  $G \leftarrow G^{up}$ ;  $\Gamma \leftarrow$  (up);
else if ( $R^{down} < R^{up}$ ) then
  If  $\Gamma =$  (down) then  $\nearrow \delta$ , otherwise  $\searrow \delta$ ;
   $\alpha \leftarrow \alpha^{down}$ ;  $G \leftarrow G^{down}$ ;  $\Gamma \leftarrow$  (down);
end if

```

3.4. Generating Starting Values and Stopping Criteria. We continue by introducing an incremental approach for finding good initial values for the iterative optimization by the ADF algorithm.

REMARK 3.9 (Stepwise increase of r). *A successful strategy for finding good initial values for the optimization is to start with minimal rank $r_0 = \dots = r_d = 1$, and each time the algorithm does not do sufficient progress anymore (cf. Remark 3.10), the ranks r_μ of G are increased until the target rank is reached. For the very first guess with TT ranks $r_1 = \dots = r_{d-1} = 1$, we define*

$$(G_s(i))_{1,1} := \frac{1}{\sqrt{n}}, \quad \forall s, i.$$

G is uniform and fulfils all required orthogonality conditions, cf. Theorem 3.4. Finally, we need a reliable stopping criterion and decide when to increase the ranks.

REMARK 3.10 (Breaking criteria). *We break if one of the following criteria is met:*

- *the last 10 directions were (back), i.e., there is no reduction of the residual even if the SOR parameter α approaches 1.*
- *the last 5 quotients of old and new residuals are in average too small, and either the direction is (down) or the change in the two last quotients of residuals is too small.*

The term "too small" is related to a parameter ε . Most reasonable choices vary between 10^{-4} and 10^{-6} . The first criterion prevents that the algorithm gets stuck trying to lower α

Algorithm 3 ADF algorithm

```

Initialize the representation  $G$  for  $r = 1$  (Remark 3.9),  $\alpha$  and  $\delta$ ;
while  $r \leq r_{final}$  do
  for  $iter = 1, \dots, iter_{max}$  do
    do the while loop lefthand, then righthand: {Remark 3.8}
    while  $\Gamma = (back)$  do
      for (up) and (down) direction optimize respective hand; {Theorem 3.4, Lemma 3.5}
      choose direction; {Algorithm 2}
    end while
    if breaking criteria apply then
      stop and continue outer for loop; {Remark 3.10}
    end if
  end for
  adapt representation to  $r + 1$ ; {Remark 3.9}
end while

```

more and more. In the second one, instead of using some kind of absolute criteria regarding the residual, it is much better to look at relative improvements. As these can fluctuate a bit we take the average of several. In order to prevent too early breaking, the direction is supposed to be (down), as while α increases (in case of (up)) or is accidentally far too large (in case of (back)), there is still a chance that this improves. However, if this happens too slow, the algorithm will break anyway to prevent that the algorithm gets stuck. The final ADF algorithm is given in Algorithm 3

4. Numerical Experiments.

4.1. Generating of Data and Details to Measurements. In order to obtain a sufficient slice density, cf. Definition 1.1, we generate the set P in a quasi-random way

as follows: For each direction $\mu = 1, \dots, d$ and each index $i_\mu \in \mathcal{I}_\mu$ we pick $C_{ov}r^2$ indices $i_1, \dots, i_{\mu-1}, i_{\mu+1}, \dots, i_d$ at random (uniformly). This gives in total $dnC_{ov}r^2$ samples (excluding some exceptions), where C_{ov} is the oversampling factor in the sense that the low rank tensor format inhibits at most dnr^2 degrees of freedom.

As a control set C we use a set of the same cardinality as P that is generated in the same way. We give neither a limit to time nor to the number of iterations and use only the previously mentioned breaking criteria with varying $\varepsilon \in \{10^{-4}, 10^{-5}, 10^{-6}\}$. For the results of the tests we denote the ratio of known points $\rho = \#P/n^d$, the relative residual $res_P = \|A - X\|_P / \|A\|_P$, the error on the control set $res_C = \|A - X\|_C / \|A\|_C$ and the *time* in seconds (s), minutes (m) or hours (h).

4.2. Approximation of a Full Rank Tensor with Decaying Singular Values.

As a first example, we consider a tensor $A \in \mathbb{R}^{\mathcal{I}}$ given by the entries

$$A_{(i_1, \dots, i_d)} := \left(\sum_{\mu=1}^d i_\mu^2 \right)^{-1/2}.$$

We carry out three different tests, each one focusing on a different parameter, i.e. d (dimension), r (final rank) and n (size).

Each combination of parameters is tested 10 times for different random P and C , where $\langle res_C \rangle$ and $\langle res_P \rangle$ denote the geometric mean of the respective results and $\langle time \rangle$ the arithmetic mean of times. A plot of the convergence of $\langle res_P \rangle, \langle res_C \rangle$ for fixed $d = 8$ and $n = 20$ is given in Figure 4.1. We observe convergence for all choices of parameters. In Table 4.1 we list the detailed results for oversampling factor $C_{ov} = 10$ and stopping criterion $\varepsilon = 10^{-6}$.

r	$\langle res_C \rangle$	$\langle res_P \rangle$	$\langle time \rangle$
2	1.94e-02	8.15e-03	14 s
3	2.05e-03	3.84e-04	1.3 m
4	1.72e-03	7.50e-05	24 m
5	1.49e-03	4.50e-05	39 m
6	2.25e-03	1.84e-05	1.7 h
7	8.53e-04	7.36e-06	2.6 h

d	$\langle res_C \rangle$	$\langle res_P \rangle$	$\langle time \rangle$
5	1.30e-02	2.07e-03	6.3 s
8	2.98e-03	4.15e-04	32 s
13	3.07e-03	6.02e-04	2.9 m
21	6.29e-03	4.03e-03	4.3 m
34	7.66e-03	7.59e-03	27 s
55	4.63e-03	4.56e-03	2.1 m

TABLE 4.1

Convergence and timing with respect to the target rank r for fixed $d = 8, n = 20, C_{ov} = 10, \varepsilon = 10^{-6}$ (left). Convergence and timing with respect to the dimension d for fixed $r = 3, n = 8, C_{ov} = 10, \varepsilon = 10^{-6}$ (right).

We observe that the timing results can be quite inhomogenous due to the stopping criterion that does not limit the maximal number of iterative steps. However, the results show that an approximation in dimension $d = 55$ still works fine, although only extremely few points of the whole tensor (less than $10^{-50} \times n^d$) are known.

At last we consider the variation of the mode sizes $n \in \{8, 16, 32\}$ in Table 4.2. Here we also observe an independence of the mode size n , but we could observe in further numerical experiments that for large n and larger ranks r the results are less satisfying.

4.3. Reconstruction of a Low Rank Tensor without Noise. As second example, we consider quasi-random tensors with exact, common low TT ranks $A \in TT(r, \dots, r)$ (cf.

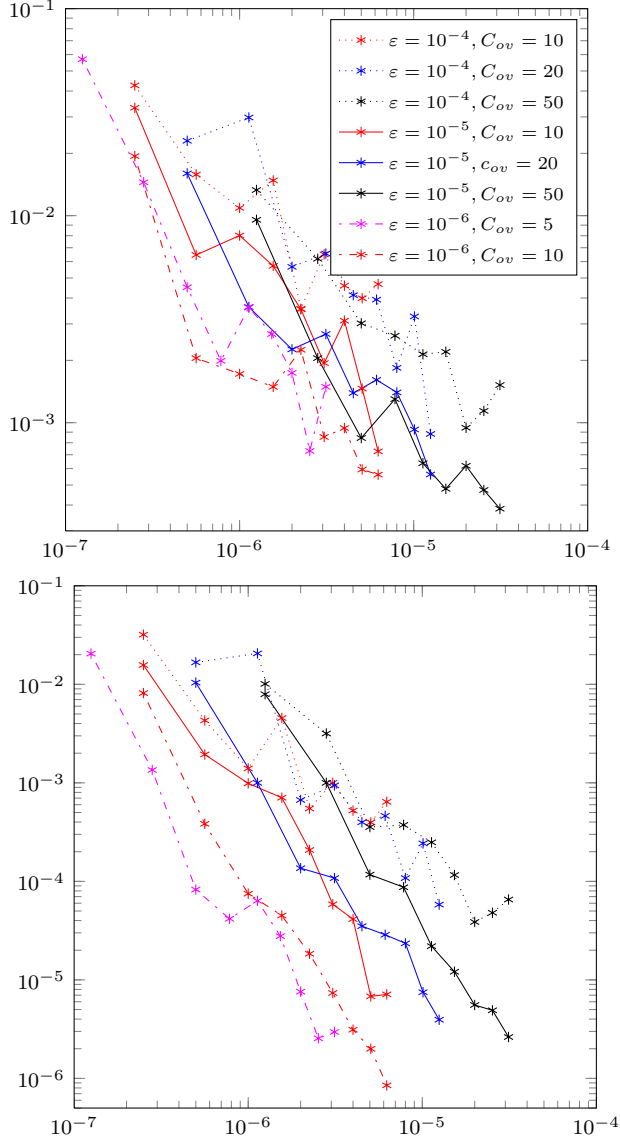


FIG. 4.1. Plotted are the residuals (res_P) (right) as well as the control residuals (res_C) (left) as function of ρ for varying target ranks $r = 2, \dots, 10$. Each curve corresponds to one choice of the oversampling parameter C_{ov} and the stopping parameter ε .

Definition 1.2). Each tensor is generated via a TT representation G as follows: Each entry of G_1, \dots, G_d is (uniformly) assigned with a random value in $[-0.5, 0.5]$. The tensor is then computed as $A = A^G$. Each combination of parameters is tested 20 times for different random P and C . We consider such a reconstruction successful if $res_C < 10^{-3}$. As an additional heuristic method we allow the algorithm after a failure to try the same task at most 5 times again. In these tests only portions of the previous P (which increase with the current rank) are used. However, no new information is anyhow used in these trials. Two diagrams, for $d = 4, 5$, with fixed $n = 20$ and $\varepsilon = 10^{-5}$ are given in Figure 4.2, displaying

n	$\langle res_C \rangle$	$\langle res_P \rangle$	$\langle time \rangle$
8	2.91e-03	1.56e-04	20 s
16	7.13e-03	3.87e-04	1.4 m
32	6.82e-03	4.01e-04	2.8 m

TABLE 4.2

Convergence and timing with respect to the mode size n for fixed $d = 8, r = 4, C_{ov} = 10, \varepsilon = 10^{-5}$.

the numbers of successes in 20 shades of gray, from white (0) to black (all 20).

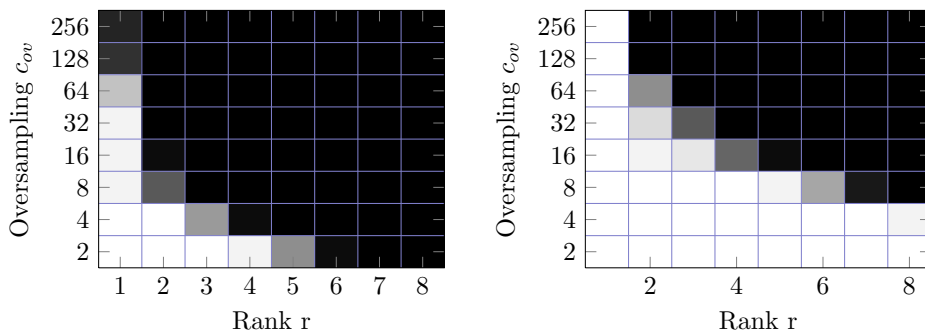


FIG. 4.2. Displayed as shades of gray (white (0) to black (all 20)) are the numbers of successful reconstructions for varying target ranks $r = 1, \dots, 8$ and oversamplings $C_{ov} = 2, 4, \dots, 256$ with $d = 4$ (left) and $d = 5$ (right)

We observe that the results for $d = 4$ are quite satisfying and that with increasing rank, less oversampling is needed. For $d = 5$, the performance is decreasing rather fast. In general the known portion of points ρ seems to effort a magnitude of about 10^{-3} to 10^{-2} .

4.4. Reconstruction of a Low Rank Tensor with Noise. As last test we exactly repeat the previous one but with perturbed tensors $\hat{A} = A + 10^{-4}\nu\mathcal{E}$, where A is generated as before and $\nu := \|A\|_P/\sqrt{\#P}$. \mathcal{E} is a tensor of same proportions; each entry being a (uniformly) quasi-randomly assigned value in $[-1, 1]$. A test is considered successful if $res_C < 10^{-3}$, where the control set residuum is still evaluated on A . However, no information about the non perturbed tensor is used in the algorithm. We desist from a diagram as there is no observable difference. It seems as if the algorithm ignores uniform noise as far as theoretically possible.

5. Conclusions. In this article we presented an alternating directions fitting algorithm that aims at finding a low tensor rank approximation to a tensor whose entries are known only in a small subset of all indices. It is important to use a certain oversampling factor in order to obtain a reasonable reconstruction of the tensor, and in our numerical experiments it turns out that this factor depends on the dimension but can be decreased with increasing rank, where it approaches $C_{ov} = 2$ in dimension $d = 4$. The SOR-type solver of the first order optimality conditions is able to minimize the residual on the known set of indices (the samples) for moderate ranks $r < 10$ and dimension $d < 50$. A modification or extension is necessary in order to treat varying TT ranks r_1, \dots, r_{d-1} instead of a uniform rank. Also, large mode sizes $n > 100$ possibly require smoothness conditions and a refined sampling strategy. The influence of noise on the reconstruction is rather harmless, where the noise can be unstructured or of rank structure but of smaller magnitude than the desired target accuracy. It seems that the low rank format introduces an automatic

regularization in the same way as the singular value truncation pronounces low frequency components.

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