## Low-rank approximate inverse for preconditioning tensor-structured linear systems<sup>\*</sup>

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#### Abstract

In this paper, we propose an algorithm for the construction of low-rank approximations of the inverse of an operator given in low-rank tensor format. The construction relies on an updated greedy algorithm for the minimization of a suitable distance to the inverse operator. It provides a sequence of approximations that are defined as the projections of the inverse operator in an increasing sequence of linear subspaces of operators. These subspaces are obtained by the tensorization of bases of operators that are constructed from successive rankone corrections. In order to handle high-order tensors, approximate projections are computed in low-rank Hierarchical Tucker subsets of the successive subspaces of operators. Some desired properties such as symmetry or sparsity can be imposed on the approximate inverse operator during the correction step, where an optimal rank-one correction is searched as the tensor product of operators with the desired properties. Numerical examples illustrate the ability of this algorithm to provide efficient preconditioners for linear systems in tensor format that improve the convergence of iterative solvers and also the quality of the resulting low-rank approximations of the solution.

## 1 Introduction

This paper is concerned with the numerical solution of high-dimensional linear systems of equations in tensor format

$$Au = b, \quad u \in \mathbb{R}^{n_1} \otimes \ldots \otimes \mathbb{R}^{n_d},\tag{1}$$

using low-rank approximation methods. These methods consist in approximating the solution under the form

$$\sum_{i_1} \dots \sum_{i_d} \alpha_{i_1 \dots i_d} w_{i_1}^1 \otimes \dots \otimes w_{i_d}^d$$

with  $w_{i_{\mu}}^{\mu} \in \mathbb{R}^{n_{\mu}}$ ,  $1 \leq \mu \leq d$ , and where the set of coefficients  $(\alpha_{i_{1}...i_{d}})$  possesses some particular structure yielding a representation with reduced complexity. When using suitable approximation formats, low-rank approximation methods result in a complexity of algorithms that grows linearly with the dimension d, thus allowing the numerical solution of high-dimensional problems (see the recent surveys [25, 7, 24, 19] and monograph [21]). Different strategies have been proposed for the construction of low-rank approximations of the solution of equations in tensor format. The first class of methods consists in defining the approximation as the minimizer in a low-rank tensor subset of some distance to the solution (e.g. the norm of the residual of equation (1)), see e.g. [5, 12]. An approximation with prescribed accuracy can be obtained by introducing an adaptive selection of tensor subsets or by using greedy constructions where corrections of the approximation are successively computed in fixed low-rank subsets (usually rank-one subsets) [2, 6, 14]. A series of improved algorithms have been proposed in order to increase the quality of suboptimal pure greedy constructions (see [32, 33, 35, 34, 30, 17] and [15] for the analysis of a large class of improved

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greedy algorithms). The second class of methods consists in using classical iterative solvers with low-rank tensor algebra, using efficient algorithms for low-rank tensor compressions [26, 27, 3].

In this paper, we are interested in the construction of low-rank preconditioners for equations in tensor format, yielding preconditioned equations

$$PAu = Pb$$

with a preserved low-rank tensor format. Preconditioning aims at improving the convergence of iterative methods but also at improving the quality of low-rank approximations defined from the residual of the equation. Different strategies have been proposed for the construction of low-rank preconditioners. In the case of equations resulting from a discretization of stochastic equations, a rank-one preconditioner has been introduced in [16]. It is based on the inverse of the expectation of the random operator, and it is particularly efficient when the random operator has a small variance. In [31], a more general rank-one preconditioner has been defined as the inverse of a rank-one approximation of the operator. This preconditioner has been exploited in [39] for the solution of equations arising from the discretization of stochastic parametric equations. In the same context, a rank-one preconditioner has also been defined in [41] as the solution of the minimization of ||I - PA|| over the set of rank-one operators P.

Rank-one preconditioners may be efficient if the operator A only slightly deviates from a rank-one operator. In order to address more general situations, different strategies have been proposed for the construction of higher rank preconditioners. In [23], a preconditioner is obtained by truncating an expansion of the inverse of the operator. In [37], a preconditioner P is defined as the best approximation of the inverse of the operator with the particular structure  $P = P^1 \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes I \otimes P^d$  corresponding to a rank-d preconditioner. More recently, an algorithm has been proposed in [36] for the construction of a low-rank preconditioner P in tensor-train format. It relies on the solution of the rank. In order to avoid the inversion of large matrices (large  $n_{\mu}$ ), a quantization technique is introduced.

In the present paper, we propose an algorithm for the computation of a low-rank approximation P of the inverse operator  $A^{-1}$  using Tucker or Hierarchical Tucker format. This algorithm is an updated greedy algorithm for the minimization of a suitable distance  $||A^{-1} - P||_{\star}$ . The norm  $|| \cdot ||_{\star}$  is chosen such that the approximation can be computed without any a priori approximation of  $A^{-1}$ , and it is chosen according to the properties of A (namely symmetric positive definite or simply definite operator). Compared to a direct minimization of  $||A^{-1} - P||_{\star}$  over a set of Tucker or Hierarchical Tucker tensors with given rank, the greedy procedure has the advantages of being adaptive and of considerably reducing the complexity of the construction of a low-rank approximation, therefore allowing the manipulation of large dimensions  $n_{\mu}$ . Starting from  $P_0 = 0$ , one step of the updated greedy algorithm consists in (i) computing a rank-one correction of the previously computed approximation  $P_{r-1}$  by minimizing  $||A^{-1} - P_{r-1} - W_r||_{\star}$  over the set of rank-one operators  $W_r = W_r^1 \otimes \ldots \otimes W_r^d$ , (ii) updating reduced spaces of operators  $\mathcal{U}_r^\mu$   $(1 \le \mu \le d)$  which are defined as the span of the set of operators  $\{W_1^\mu, \ldots, W_r^\mu\}$ , and (iii) computing a new approximation  $P_r$  in the space  $\mathcal{U}_r = \mathcal{U}_r^1 \otimes \ldots \otimes \mathcal{U}_r^d$  by minimizing  $||A^{-1} - P_r||_{\star}$  in  $\mathcal{U}_r$  or over a set of low-rank Hierarchical Tucker tensors in  $\mathcal{U}_r$ . More precisely, the approximation  $P_r$  is searched under the form

$$P_r = \sum_{i_1=1}^r \dots \sum_{i_d=1}^r \alpha_{i_1,\dots,i_d} W_{i_1}^1 \otimes \dots \otimes W_{i_d}^d,$$

where the set of coefficients  $\alpha$  is optimized in  $\mathbb{R}^r \otimes \ldots \otimes \mathbb{R}^r$  or in a low-rank Hierarchical Tucker subset of  $\mathbb{R}^r \otimes \ldots \otimes \mathbb{R}^r$ . For the solution of the minimization problems over the set of rank-one tensors (step (i)) and the set of Hierarchical Tucker tensors with bounded rank (step (iii)), alternating minimization algorithms are used [28, 40].

Some desired properties such as symmetry and sparsity can be imposed on the approximate inverse. This is done in the correction step (i) where the optimal rank-one correction is searched as the tensor product of operators with the desired properties. During the alternating minimization algorithm, imposing the symmetry on the matrix  $W_r^{\mu}$  requires the solution of a Sylvester equation.

For imposing sparsity on  $W_r^{\mu}$ , we propose a straightforward generalization of the sparse approximate inverse algorithm proposed in [20], which is an adaptive algorithm for the determination of the sparsity pattern.

The outline of the paper is as follows. In Section 2, we briefly recall some useful definitions on tensor spaces and low-rank tensor approximations. In Section 3, we introduce an algorithm for computing a rank-one approximation of the inverse operator, with possible imposed properties. In Section 4, we introduce the algorithm for computing a low-rank approximate inverse in low-rank Tucker or Hierarchical Tucker formats. In Section 5, the efficiency of the proposed preconditioning technique is illustrated on numerical problems: a Poisson equation in high dimension (symmetric problem) and a linear equation resulting from the discretization of a stochastic partial differential equation using spectral stochastic methods.

## 2 Tensor spaces and low-rank tensor approximation

#### 2.1 Tensor spaces

Let  $D = \{1, \ldots, d\}$ , with  $d \in \mathbb{N}^*$ . Let  $\mathcal{X}^{\mu}$ ,  $\mu \in D$ , be a finite dimensional space equipped with an inner product  $\langle \cdot, \cdot \rangle_{\mu}$  and the associated norm  $\|\cdot\|_{\mu}$ . We consider the tensor space  $\mathcal{X} = \mathcal{X}^1 \otimes \ldots \otimes \mathcal{X}^d$ . In the following, the simplified notation  $\bigotimes_{\mu}$  will be used for  $\bigotimes_{\mu \in D}$ , as well as  $\bigotimes_{\mu \neq \lambda}$  for  $\bigotimes_{\mu \in D \setminus \{\lambda\}}$ ,  $\lambda \in D$ . A tensor  $x \in \mathcal{X}$  can be written under the form  $x = \sum_{i=1}^r \bigotimes_{\mu} x_i^{\mu}$  for some  $r \in \mathbb{N}$  and  $x_i^{\mu} \in \mathcal{X}^{\mu}$ . The minimal integer r which allows to represent x exactly under this form is called the (canonical) rank of x.  $\mathcal{X}$  is a Hilbert space for the induced inner product  $\langle \cdot, \cdot \rangle$  defined for rank-one tensors by  $\langle \bigotimes_{\mu} x^{\mu}, \bigotimes_{\mu} y^{\mu} \rangle = \prod_{\mu \in D} \langle x^{\mu}, y^{\mu} \rangle_{\mu}$ , and extended by linearity to the whole space  $\mathcal{X}$ . The associated norm is noted  $\|\cdot\|$ .

For  $\mathcal{X}^{\mu} = \mathbb{R}^{n_{\mu}}$ , we use the vector 2-norm  $\|\cdot\|_{\mu}$  and the associated canonical inner product  $\langle \cdot, \cdot \rangle_{\mu}$ . For  $\mathcal{X}^{\mu} = \mathbb{R}^{n_{\mu} \times n_{\mu}}$ , we take for  $\|\cdot\|_{\mu}$  the Frobenius norm and for  $\langle \cdot, \cdot \rangle_{\mu}$  the associated inner product defined by  $\langle A^{\mu}, B^{\mu} \rangle_{\mu} = \operatorname{tr}((A^{\mu})^{T}B^{\mu})$  for  $A^{\mu}, B^{\mu} \in \mathbb{R}^{n_{\mu} \times n_{\mu}}$ . A matrix  $A^{\mu} \in \mathbb{R}^{n_{\mu} \times n_{\mu}}$  is identified with the corresponding operator  $A^{\mu} : \mathbb{R}^{n_{\mu}} \to \mathbb{R}^{n_{\mu}}$ , and a tensor  $A \in \bigotimes_{\mu} \mathbb{R}^{n_{\mu} \times n_{\mu}}$  is identified with the corresponding operator  $A : \bigotimes_{\mu} \mathbb{R}^{n_{\mu}} \to \bigotimes_{\mu} \mathbb{R}^{n_{\mu}}$ . We denote by  $A^{T}$  the adjoint of A for the induced inner product, which for  $A = \sum_{i=1}^{r} \bigotimes_{\mu} A^{\mu}_{i}$  is obtained by  $A^{T} = \sum_{i=1}^{r} \bigotimes_{\mu} (A^{\mu}_{i})^{T}$ , where  $(A^{\mu}_{i})^{T}$  denotes the transpose of matrix  $A^{\mu}_{i}$ .

#### 2.2 Low-rank tensor approximation

Let  $\mathcal{M} \subset \mathcal{X}$  be a subset of low-rank tensors in  $\mathcal{X}$ . The best approximation of y in  $\mathcal{M}$ , if it exists, is defined by

$$\min_{x \in \mathcal{M}} \|y - x\|$$

We also define a quasi-best approximation of y in  $\mathcal{M}$  as an element  $x^{\gamma} \in \mathcal{M}$  satisfying

$$\|y - x^{\gamma}\| \le \gamma \inf_{x \in \mathcal{M}} \|y - x\|$$

for some factor  $\gamma > 1$ . Note that a quasi-best approximation exists for any  $\gamma > 1$ .

#### 2.2.1 Canonical format

The subset of rank-r canonical tensors is defined by

$$\mathcal{C}_r(\mathcal{X}) = \left\{ x = \sum_{i=1}^r \bigotimes_{\mu} x_i^{\mu}; \ x_i^{\mu} \in \mathcal{X}^{\mu}, \ \forall \mu \in D \right\}.$$

This format is simple. However, the set  $C_r(\mathcal{X})$  is not closed for d > 2 and r > 1, therefore the best approximation problem using canonical format is ill-posed in this case [10]. Alternating minimization algorithm [25] or other optimization algorithms [1, 11] can be used to solve the approximation problem in  $C_r(\mathcal{V})$ . However, for d > 2, there is no available algorithm for computing a quasi-best approximation in  $C_r(\mathcal{X})$  with a controlled factor  $\gamma$ .

#### 2.2.2 Tucker format

The subset of Tucker tensors with rank  $r = (r_{\mu})_{\mu \in D}$ , introduced in [38], is defined by

$$\mathcal{T}_{r}(\mathcal{X}) = \left\{ x \in \mathcal{X}; \text{ there exist linear subspaces } \mathcal{U}^{\mu} \text{ with} \\ dim(\mathcal{U}^{\mu}) = r_{\mu}, \ 1 \le \mu \le d, \text{ such that } x \in \bigotimes_{\mu=1}^{d} \mathcal{U}^{\mu} \right\}.$$
(2)

Letting  $\mathcal{I}_r = \mathcal{I}_{r_1} \times \ldots \times \mathcal{I}_{r_d}$  with  $\mathcal{I}_{r_\mu} = \{1, \ldots, r_\mu\}$ , it is equivalently defined by

$$\mathcal{T}_{r}(\mathcal{X}) = \left\{ x = \sum_{i \in \mathcal{I}_{r}} \alpha_{i} \bigotimes_{\mu} x_{i_{\mu}}^{\mu} ; \; \alpha \in \bigotimes_{\mu=1}^{d} \mathbb{R}^{r_{\mu}}, \; x_{i_{\mu}}^{\mu} \in \mathcal{X}^{\mu} \right\},$$
(3)

where  $\alpha$  is the so called core tensor of the Tucker representation. The set  $\mathcal{T}_r(\mathcal{X})$  is closed [13], so that a best approximation problem of a tensor in  $\mathcal{T}_r(\mathcal{X})$  always exists. Moreover, when using the canonical norm, the Higher Order Singular Value Decomposition (HOSVD) algorithm proposed in [8] allows the efficient computation of a quasi-best approximation of a tensor with a controlled factor  $\gamma = \sqrt{d}$ . This quasi-best approximation can further be improved using Higher Order Orthogonal Iterations (HOOI) algorithm [9], which is an alternating minimization algorithm. The drawback of this format is that the core tensor  $\alpha$  is of order d so that this format suffers from the curse of dimensionality.

#### 2.2.3 Hierarchical Tucker format

The Hierarchical Tucker tensor format has been introduced in [22] and is defined as follows. Let T be a tree of dimensions, defined as a full binary tree on D with root D. The set of leaves of the tree is defined by  $L(T) = \{\{\mu\}; \mu \in D\}$  and the set of interior nodes is  $I(T) = T \setminus L(T)$ . The set of successors S(t) of an interior note  $t \in I(T)$  is composed by two nonempty successors  $t_1$  and  $t_2$  in T such that  $t = t_1 \cup t_2$  and  $t_1 \cap t_2 = \emptyset$ . The complement of  $t \in T$  is denoted by  $t^c = D \setminus t$ . We denote by  $\mathcal{X}^t = \bigotimes_{\mu \in t} \mathcal{X}^{\mu}$  and  $\mathcal{X}^{t^c} = \bigotimes_{\mu \in t^c} \mathcal{X}^{\mu}$ . The t-matricization operator  $M_t : \mathcal{X} \to \mathcal{X}^t \otimes \mathcal{X}^{t^c}$  is defined for  $x = \sum_{i=1}^r \bigotimes_{\mu} x_i^{\mu}$  by

$$M_t(x) = \sum_{i=1}^r \left(\bigotimes_{\mu \in t} x_i^{\mu}\right) \otimes \left(\bigotimes_{\mu \in t^c} x_i^{\mu}\right)$$

The *t*-rank of *x* is then defined as the rank of the 2-order tensor  $M_t(x) \in \mathcal{X}^t \otimes \mathcal{X}^{t^c}$ . Given a tree of dimensions *T* and a family of ranks  $r = (r_t)_{t \in T}$  associated with the tree, the set of Hierarchical Tucker tensors with bounded rank *r* is defined by

$$\mathcal{H}_r^T(\mathcal{X}) = \{ x \in \mathcal{X}; \ t\text{-rank}(x) \le r_t, \ \forall t \in T \}.$$

We note that the set of Tucker tensors  $\mathcal{T}_{(r_1,...,r_d)} = \{x \in \mathcal{X}; \ \mu\text{-rank}(x) \leq r_{\mu}, \ \forall \mu \in D\}$ , and therefore

$$\mathcal{H}_r^T(\mathcal{X}) \subset \mathcal{T}_{(r_1,\ldots,r_d)}(\mathcal{X}).$$

In practice, a tensor  $x \in \mathcal{H}_r^T(\mathcal{X})$  can be represented under the form

$$x = \sum_{i=1}^{r_{t_1}} \sum_{j=1}^{r_{t_2}} \beta_{ij}^D x_i^{t_1} \otimes x_j^{t_2}, \ \beta^D \in \mathbb{R}^{r_{t_1} \times r_{t_2}}, \ \{t_1, t_2\} = S(D),$$

where for all  $t \in I(T) \setminus \{D\}$ ,

$$x_k^t = \sum_{i=1}^{r_{t_1}} \sum_{j=1}^{r_{t_2}} \beta_{ijk}^t x_i^{t_1} \otimes x_j^{t_2}, \ \beta^t \in \mathbb{R}^{r_{t_1} \times r_{t_2} \times r_t}, \ \{t_1, t_2\} = S(t), \ k \in \{1, \dots, r_t\}$$

Therefore,  $x \in \mathcal{H}_r^T(\mathcal{X})$  is completely determined by the set of transfer tensors  $\{\beta^t; t \in I(T)\}$ associated with the interior nodes of the tree, and the set of elements  $\{x_i^{\mu}; i \in \mathcal{I}_{r_{\mu}}, \mu \in D\}$ associated with the leaves of the tree. The tensor x can be written

$$x = \sum_{i \in \mathcal{I}_{r_1} \times \ldots \times \mathcal{I}_{r_d}} \alpha_i \bigotimes_{\mu=1}^d x_{i_{\mu}}^{\mu},$$

where the tensor  $\alpha \in \mathcal{H}_r^T(\bigotimes_{\mu=1}^d \mathbb{R}^{r_\mu})$  is a rank-*r* Hierarchical Tucker tensor that can be expressed in terms of the transfer tensors  $\{\beta^t; t \in I(T)\}$ .

The set  $\mathcal{H}_r^T(\mathcal{X})$  is closed (see [21], section 11.4.1.1) so that a best approximation of a tensor in  $\mathcal{H}_r^T(\mathcal{X})$  always exists. Moreover, when using the induced canonical norm, the Hierarchical Singular Value Decomposition (HSVD) algorithm proposed in [18] allows the efficient computation of a quasi-best approximation of a tensor in  $\mathcal{H}_r^T(\mathcal{X})$  with a controlled factor  $\gamma = \sqrt{2d-3}$ . Besides, given that #I(T) = d-1 and #L(T) = d, the Hierarchical Tucker format does not suffer from the curse of dimensionality since the dimension of the parametrization of a tensor in  $\mathcal{H}_r^T(\mathcal{X})$  depends linearly on d.

## **3** Rank-one approximation of an inverse operator

Let consider A in  $\mathcal{W} = \bigotimes_{\mu=1}^{d} \mathcal{W}^{\mu}$ , with  $\mathcal{W}^{\mu} = \mathbb{R}^{n_{\mu} \times n_{\mu}}$ . In this section, we introduce an algorithm for computing a rank-one approximation of the inverse  $A^{-1}$  of A, considered as an operator from  $\bigotimes_{\mu=1}^{d} \mathbb{R}^{n_{\mu}}$  to  $\bigotimes_{\mu=1}^{d} \mathbb{R}^{n_{\mu}}$ . The rank-one approximation is searched in a linear subspace  $\mathcal{U} = \bigotimes_{\mu=1}^{d} \mathcal{U}^{\mu}$  of  $\mathcal{W}$ , with  $\mathcal{U}^{\mu} = \mathcal{W}^{\mu}$  or  $\mathcal{U}^{\mu} \subset \mathcal{W}^{\mu}$ , a linear subspace of operators with prescribed properties such as symmetry or sparsity.

#### 3.1 Best rank-one correction

Let  $P \in \mathcal{W}$  be a first approximation of  $A^{-1}$  (e.g. a known preconditioner of A).  $\mathcal{C}_1(\mathcal{U})$  denotes the set of rank-one elements of the tensor space  $\mathcal{U} \subset \mathcal{W}$ . The best rank-one correction  $W = \bigotimes_{\mu=1}^{d} W^{\mu} \in \mathcal{C}_1(\mathcal{U})$  of P is defined by the following problem

$$\min_{W \in \mathcal{C}_1(\mathcal{U})} \|A^{-1} - (P + W)\|_{\star}$$
(4)

where  $\|\cdot\|_{\star}$  is a norm on  $\mathcal{W}$  that has to be chosen such that an approximation W can be computed without knowing  $A^{-1}$ .

#### 3.2 Definition of the norm $\|\cdot\|_{\star}$

If A is symmetric positive definite, we choose the norm  $\|\cdot\|_{\star} = \|\cdot\|_A$  defined by  $\|X\|_A = \|XA^{1/2}\| = \sqrt{\langle XA, X \rangle}$  and associated with the inner product  $\langle \cdot, \cdot \rangle_A$  defined by  $\langle X, Y \rangle_A = \langle XA, Y \rangle$ . We note that  $\|A^{-1} - (P+W)\|_A = \|I - (P+W)A\|_{A^{-1}}$ , so that the minimization problem (4) provides a left approximate inverse (P+W) of A.<sup>1</sup>

In the more general case of a *definite operator* A, we choose the norm  $\|\cdot\|_{\star} = \|\cdot\|_{AA^T}$  defined by  $\|X\|_{AA^T} = \|XA\| = \sqrt{\langle XA, XA \rangle} = \sqrt{\langle XAA^T, X \rangle}$  and associated with the inner product

<sup>&</sup>lt;sup>1</sup>We could also choose  $\|\cdot\|_{\star} = \|\cdot\|_A$  with  $\|X\|_A = \|A^{1/2}X\| = \sqrt{\langle AX, X \rangle}$ , so that the minimization of  $\|A^{-1} - (P+W)\|_{\star} = \|I - A(P+W)\|_{A^{-1}}$  provides a right approximate inverse (P+W) of A.

 $\langle \cdot, \cdot \rangle_{AA^T}$  defined by  $\langle X, Y \rangle_{AA^T} = \langle XA, YA \rangle = \langle XAA^T, Y \rangle$ . We note that  $||A^{-1} - (P+W)||_{AA^T} = ||I - (P+W)A||$ , so that the minimization problem (4) provides a left approximate inverse (P+W) of A.<sup>2</sup>

From now on, we consider that  $\|\cdot\|_{\star} = \|\cdot\|_{AB}$ , with B = I if A is symmetric positive definite or  $B = A^T$  if A is simply definite, and we denote by  $\langle \cdot, \cdot \rangle_{\star} = \langle \cdot, \cdot \rangle_{AB}$  the associated inner product on  $\mathcal{W}$ .

#### 3.3 Stationarity conditions

A necessary condition of optimality for a solution  $W = \bigotimes_{\mu=1}^{d} W^{\mu}$  of problem (4) is

$$\langle A^{-1} - (P+W), \delta W \rangle_{\star} = 0, \quad \forall \delta W \in T_W(\mathcal{C}_1(\mathcal{U})),$$
(5)

where  $T_W(\mathcal{C}_1(\mathcal{U}))$  is the tangent space of  $\mathcal{C}_1(\mathcal{U})$  at W defined by

$$T_W(\mathcal{C}_1(\mathcal{U})) = \sum_{\mu=1}^d T_W^{(\mu)}(\mathcal{C}_1(\mathcal{U})) \subset \mathcal{C}_d(\mathcal{U}),$$

with

$$T_W^{(\mu)}(\mathcal{C}_1(\mathcal{U})) = \left\{ \delta W = W^1 \otimes \ldots \otimes \delta W^\mu \otimes \ldots \otimes W^d \in \mathcal{C}_1(\mathcal{U}); \delta W^\mu \in \mathcal{U}^\mu \right\}$$

Using the definition of inner product  $\langle \cdot, \cdot \rangle_{\star} = \langle \cdot, \cdot \rangle_{AB}$ , we have that W satisfies (5) if and only if

$$\langle B - (P + W)AB, \delta W \rangle = 0, \quad \forall \delta W \in T_W(\mathcal{C}_1(\mathcal{U})).$$
 (6)

Let  $\mathscr{P}^{\mu} : \mathscr{W}^{\mu} \to \mathscr{U}^{\mu}, \ \mu \in D$ , denote the orthogonal projector from  $\mathscr{W}^{\mu}$  into  $\mathscr{U}^{\mu}$ , such that  $\mathscr{P}^{\mu}\mathscr{P}^{\mu} = \mathscr{P}^{\mu}$  and  $\langle \mathscr{P}^{\mu}(X^{\mu}), Y^{\mu} - \mathscr{P}^{\mu}(Y^{\mu}) \rangle_{\mu} = 0$  for all  $X^{\mu}, Y^{\mu} \in \mathscr{W}^{\mu}$ . The operator  $\mathscr{P} : \mathscr{W} \to \mathscr{U}$  defined by  $\mathscr{P} = \bigotimes_{\mu=1}^{d} \mathscr{P}^{\mu}$  is the orthogonal projector from  $\mathscr{W}$  to  $\mathscr{U}$  such that  $\mathscr{P}\mathscr{P} = \mathscr{P}$  and

$$\langle \mathscr{P}(X), Y - \mathscr{P}(Y) \rangle = 0, \quad \forall X, Y \in \mathcal{W}.$$
 (7)

Noting that  $T_W(\mathcal{C}_1(\mathcal{U})) \subset \mathcal{U}$ , we have that for all  $\delta W \in T_W(\mathcal{C}_1(\mathcal{U}))$ ,

$$\langle B - (P+W)AB, \delta W \rangle = \langle B - (P+W)AB, \mathscr{P}(\delta W) \rangle$$
  
=  $\langle \mathscr{P}(B - (P+W)AB), \mathscr{P}(\delta W) \rangle$   
=  $\langle \mathscr{P}(B - (P+W)AB), \delta W \rangle.$ 

Therefore, using the definition of the tangent space  $T_W(\mathcal{C}_1(\mathcal{U}))$ , we obtain that W satisfies (6) if and only if for all  $\lambda \in D$ ,

$$\langle \mathscr{P}(WAB), \delta W \rangle = \langle \mathscr{P}(R(P)), \delta W \rangle, \quad \forall \delta W \in T_W^{(\lambda)}(\mathcal{C}_1(\mathcal{U})), \tag{8}$$

with R(P) = B - PAB.

#### 3.4 Alternating minimization algorithm

For solving (4), we use an alternating minimization algorithm. Starting from an arbitrary initialization  $W = \bigotimes_{\mu} W^{\mu} \in \mathcal{C}_1(\mathcal{U})$ , it consists in solving successively the quadratic optimization problems

$$\min_{W^{\lambda} \in \mathcal{U}^{\lambda}} \|A^{-1} - P - \bigotimes_{\mu=1}^{d} W^{\mu}\|_{\star}^{2},$$
(9)

<sup>&</sup>lt;sup>2</sup>We could also choose  $||X||_{\star} = ||AX|| = \sqrt{\langle AX, AX \rangle}$ , so that the minimization of  $||A^{-1} - (P + W)||_{\star} = ||I - A(P + W)||$  provides a right approximate inverse P + W of A.

for  $\lambda \in \{1, \ldots, d, 1, \ldots\}$ . It is observed that this algorithm converges to an element W that satisfies the stationarity condition (5), or equivalently (8) for all  $\lambda \in D$ . However, note that it does not necessarily yield a solution of (4).

The solution of (9) is equivalent to the solution of Equation (8) for given  $W^{\mu}$ ,  $\mu \neq \lambda$ . Therefore, noting  $C = AB = \sum_{i=1}^{r_C} \otimes_{\mu} C_i^{\mu}$  and  $R(P) = B - PAB = \sum_{i \in \mathcal{I}_{r_R}} \gamma_i \otimes_{\mu} R_{i_{\mu}}^{\mu}$ , we obtain that (9) is equivalent to the following linear problem on  $W^{\lambda} \in \mathcal{W}^{\lambda}$ :

$$\mathscr{P}^{\lambda}(W^{\lambda}Q^{\lambda}) = \mathscr{P}^{\lambda}(H^{\lambda}(P)), \tag{10}$$

with

$$Q^{\lambda} = \sum_{i=1}^{r_C} C_i^{\lambda} \prod_{\mu \neq \lambda} \left\langle \mathscr{P}^{\mu}(W^{\mu}C_i^{\mu}), W^{\mu} \right\rangle_{\mu}, \qquad (11)$$

$$H^{\lambda}(P) = \sum_{i \in \mathcal{I}_{r_R}} R^{\lambda}_{i_{\lambda}} \gamma_i \prod_{\mu \neq \lambda} \left\langle \mathscr{P}^{\mu}(R^{\mu}_{i_{\mu}}), W^{\mu} \right\rangle_{\mu}.$$
 (12)

If  $\mathcal{U}^{\lambda} = \mathcal{W}^{\lambda}$ , that means if we do not impose any particular property to matrices associated with dimension  $\lambda$ , then  $\mathscr{P}^{\lambda}$  is the identity on  $\mathcal{W}^{\lambda}$  and Equation (10) becomes

$$W^{\lambda}Q^{\lambda} = H^{\lambda}(P), \tag{13}$$

with  $Q^{\lambda}$  and  $H^{\lambda}(P)$  defined in Equations (11) and (12) respectively.

#### 3.5 Imposing properties

#### 3.5.1 Imposing symmetries

We note  $D_{sym}$ ,  $D_{skew}$  and  $D_c$  three sets of indices such that they form a partition of  $D = \{1, \ldots, d\}$ . Then, we consider  $\mathcal{U} = \bigotimes_{\mu} \mathcal{U}^{\mu}$  such that

$$\mathcal{U}^{\mu} = \begin{cases} \{X \in \mathcal{W}^{\mu}; \ X = X^{T}\} & \text{if } \mu \in D_{sym}, \\ \{X \in \mathcal{W}^{\mu}; \ X = -X^{T}\} & \text{if } \mu \in D_{skew}, \\ \mathcal{W}^{\mu} & \text{if } \mu \in D_{c}. \end{cases}$$

The orthogonal projector  $\mathscr{P}^{\mu}: \mathcal{W}^{\mu} \to \mathcal{U}^{\mu}$  is such that

$$\mathscr{P}^{\mu}(X) = \begin{cases} \frac{1}{2}(X + X^T) & \text{if } \mu \in D_{sym}, \\ \frac{1}{2}(X - X^T) & \text{if } \mu \in D_{skew}, \\ X & \text{if } \mu \in D_c. \end{cases}$$

Therefore, the linear equation (10) in  $W^{\lambda} \in \mathcal{U}^{\lambda}$  can be written

$$\begin{cases} W^{\lambda}Q^{\lambda} + (Q^{\lambda})^{T} W^{\lambda} = H^{\lambda} + (H^{\lambda})^{T} & \text{if } \lambda \in D_{sym}, \\ W^{\lambda}Q^{\lambda} - (Q^{\lambda})^{T} W^{\lambda} = H^{\lambda} - (H^{\lambda})^{T} & \text{if } \lambda \in D_{skew}, \\ W^{\lambda}Q^{\lambda} = H^{\lambda}, & \text{otherwise.} \end{cases}$$

We notice that the equations associated with  $\lambda$  in  $D_{sym}$  or  $D_{skew}$  are particular cases of the so called Sylvester equation which can be solved with the algorithm from [4].

If A and P are symmetric, and if  $D_{sym} = D$  (that means that we search for a symmetric rank-one approximation), then  $Q^{\lambda}$  is symmetric and (10) is a continuous Lyapunov equation

$$W^{\lambda}Q^{\lambda} + Q^{\lambda}W^{\lambda} = H^{\lambda} + (H^{\lambda})^{T}.$$

#### 3.5.2 Imposing sparsity

Here, we are interested in using sparse approximation in order to handle large matrices. For  $\lambda \in D$ , let  $I^{\lambda} \subset \{1, \ldots, n_{\lambda}\}^2$  and let  $\mathcal{U}^{\lambda}$  be the subspace of matrices with sparsity pattern  $I^{\lambda}$ :

$$\mathcal{U}^{\lambda} = \left\{ X \in \mathcal{W}^{\lambda}; (X)_{kj} = 0, \ \forall (k,j) \notin I^{\lambda} \right\}.$$

The orthogonal projector from  $\mathcal{W}^{\lambda}$  onto  $\mathcal{U}^{\lambda}$  is defined for  $X^{\lambda} \in \mathcal{W}^{\lambda}$  by

$$(\mathscr{P}^{\lambda}(X^{\lambda}))_{kj} = \begin{cases} (X^{\lambda})_{kj} & \text{if } (k,j) \in I^{\lambda}, \\ 0 & \text{if } (k,j) \notin I^{\lambda}. \end{cases}$$

Similarly to the SParse Approximate Inverse (SPAI) method from [20], we reformulate equation (10) as the following minimization problem:

$$\min_{W^{\lambda} \in \mathcal{U}^{\lambda}} \left\| \mathscr{P}^{\lambda} (W^{\lambda} Q^{\lambda} - H^{\lambda}) \right\|_{\lambda}^{2}.$$
(14)

Noting  $\{w_k^{\lambda}\}_{1 \leq k \leq n_{\lambda}}$  (resp.  $\{h_k^{\lambda}\}_{1 \leq k \leq n_{\lambda}}$ ) the rows of  $W^{\lambda}$  (resp.  $H^{\lambda}$ ), we have

$$\left\|\mathscr{P}^{\lambda}(W^{\lambda}Q^{\lambda}-H^{\lambda})\right\|_{\lambda}^{2}=\sum_{k=1}^{n_{\lambda}}\left\|w_{k}^{\lambda}Q^{\lambda}P_{k}^{\lambda}-h_{k}^{\lambda}P_{k}^{\lambda}\right\|_{\lambda}^{2},$$

where  $P_k^{\lambda} \in \mathbb{R}^{n_{\lambda} \times n_{\lambda}}$  is a boolean diagonal matrix such that  $(P_k^{\lambda})_{jj} = 1$  if  $j \in I_k^{\lambda}$  and  $(P_k^{\lambda})_{jj} = 0$  if  $j \notin I_k^{\lambda}$ , where  $I_k^{\lambda} = \{j; (k, j) \in I^{\lambda}\}$  denotes the pattern of the row k. Therefore, the minimization problem (14) is equivalent to  $n_{\lambda}$  independent minimization problems (that can be solved in parallel)

$$\min_{w_k^\lambda \in \mathbb{R}^{n_\lambda}} \left\| w_k^\lambda Q^\lambda P_k^\lambda - h_k^\lambda P_k^\lambda \right\|_{\lambda}^2 \quad \text{submitted to } (w_k^\lambda)_j = 0 \text{ for all } j \notin I_k^\lambda.$$
(15)

Each problem (15) can be rewritten as the minimization of  $\|\widehat{w}_k^{\lambda}\widehat{Q}_k^{\lambda} - \widehat{h}_k^{\lambda}\|_{\lambda}^2$  over  $\widehat{w}_k^{\lambda} \in \mathbb{R}^{m_k^{\lambda}}$ , with  $m_k^{\lambda} = \#I_k^{\lambda}$ , where  $\widehat{w}_k^{\lambda}$  (resp.  $\widehat{h}_k^{\lambda}$ ) denotes the vector of non zero entries of  $w_k^{\lambda}$  (resp.  $h_k^{\lambda}P_k^{\lambda}$ ). This minimization problem on  $\widehat{w}_k^{\lambda}$  can be solved using a QR decomposition of the reduced matrix  $\widehat{Q}_k^{\lambda}$  (see [20]).

For the adaptive selection of the pattern  $I^{\lambda}$ , we use the iterative method proposed in [20]. Let  $\mathscr{P}^{\lambda,(i)}$  be the projector associated to the set of patterns  $\{I_k^{\lambda,(i)}\}_{1 \leq k \leq n_{\lambda}}$ . We start from an initial projector  $\mathscr{P}^{\lambda,(0)}$  (e.g. associated with diagonal patterns  $I_k^{\lambda,(0)} = \{k\}$ ). Then, for  $i = 0, \ldots, i_{\max}$ , we proceed as follows. We compute

$$W^{\lambda,(i)} = \arg\min_{W^{\lambda} \in \mathcal{U}^{\lambda}} \left\| \mathscr{P}^{\lambda,(i)} (W^{\lambda} Q^{\lambda} - H^{\lambda}) \right\|_{\lambda}^{2}.$$

Then, for each row k, we compute a new index

$$j_k^{\lambda,(i)} = \arg\min_{1 \le j \le n_\lambda} \left( \min_{\gamma \in \mathbb{R}} \left\| (w_k^{\lambda,(i)} + \gamma(e_j^\lambda)^T) Q^\lambda - h_k^\lambda \right\|_\lambda^2 \right),$$

where  $e_j^{\lambda}$  is the *j*-th canonical basis vector in  $\mathbb{R}^{n_{\lambda}}$ , and we set  $I_k^{\lambda,(i+1)} = I_k^{\lambda,(i)} \cup \{j_k^{\lambda,(i)}\}$ .

# 4 A constructive algorithm using projections in reduced spaces

Here, we introduce a constructive algorithm for the approximation of the inverse  $A^{-1}$  of an operator A using Tucker or Hierarchical Tucker tensor format.

The algorithm starts with an initialization  $P_0$ , such as  $P_0 = 0$  or a first approximation of  $A^{-1}$ . Knowing an approximation  $P_{r-1}$  of  $A^{-1}$ , we look for a rank-one correction  $W_r = \bigotimes_{\mu} W_r^{\mu}$  which solves

$$\min_{W \in \mathcal{C}_1(\mathcal{W})} \left\| A^{-1} - P_{r-1} - W \right\|_{\star},\tag{16}$$

where the norm  $\|\cdot\|_{\star}$  has been defined in Section 3.2. Then, we define the linear subspace

$$\mathcal{U}_r = \bigotimes_{\mu=1}^d \mathcal{U}_r^{\mu} \quad \text{with} \quad \mathcal{U}_r^{\mu} = \operatorname{span} \{W_1^{\mu}, \dots, W_r^{\mu}\}.$$

The dimension of  $\mathcal{U}_r$  is  $\prod_{\mu} r_{\mu}$ , with  $r_{\mu} \leq r$ . In practice, we construct orthogonal bases  $\{Q_i^{\mu}\}_{1 \leq i \leq r_{\mu}}$  of the subspaces  $\mathcal{U}_r^{\mu}$ , yielding a basis  $\{\bigotimes_{\mu} Q_i^{\mu}\}_{i \in \mathcal{I}_r}$  of  $\mathcal{U}_r$ , with  $\mathcal{I}_r = \{(i_1, \ldots, i_d) \in \mathbb{N}^d; 1 \leq i_{\mu} \leq r_{\mu}\}$ . The approximation  $P_r$  is then searched in the subspace  $\mathcal{U}_r$  under the form

$$P_r = \sum_{i \in \mathcal{I}_r} \alpha_i \bigotimes_{\mu=1}^d Q_i^{\mu}.$$
 (17)

If the dimension  $\mathcal{U}_r$  is sufficiently small,  $P_r$  is defined as the projection of  $A^{-1}$  on the subspace  $\mathcal{U}_r$  with respect to the inner product norm  $\|\cdot\|_{\star}$ ,

$$P_r = \arg\min_{P \in \mathcal{U}_r} \left\| A^{-1} - P \right\|_{\star},$$

and  $P_r$  is given under the form (17) with  $\alpha$  solution of the linear system

$$\sum_{i \in \mathcal{I}_r} \left\langle Q_i, Q_j \right\rangle_\star \alpha_i = \left\langle A^{-1}, Q_j \right\rangle_\star, \quad \forall j \in \mathcal{I}_r.$$

When the dimension of  $\mathcal{U}_r$  is large (e.g. for large d or large r), the computation of the projection in  $\mathcal{U}_r$  may be prohibitive. In this case, we replace the projection in  $\mathcal{U}_r$  by an approximate projection using Hierarchical Tucker format. More precisely, given a tree of dimensions T and a set of ranks  $(r_t)_{t\in T}$ , we introduce the subset of Hierarchical Tucker tensors  $\mathcal{H}_r^T(\mathcal{U}_r)$  in  $\mathcal{U}_r$ . Then, an approximation  $P_r$  is computed by solving the minimization problem

$$\min_{P \in \mathcal{H}_r^T(\mathcal{U}_r)} \left\| A^{-1} - P \right\|_{\star}$$

which is equivalent to computing an approximation  $P_r$  under the form (17) with  $\alpha$  in  $\mathcal{H}_r^T(\bigotimes_{\mu} \mathbb{R}^{r_{\mu}})$  solution of

$$\min_{\alpha \in \mathcal{H}_r^T(\bigotimes_{\mu} \mathbb{R}^{r_{\mu}})} \left\| A^{-1} - \sum_{i \in \mathcal{I}_r} \alpha_i \bigotimes_{\mu} Q_i^{\mu} \right\|_{\star}.$$

This optimization problem is solved using an alternating minimization algorithm which consists in successively minimizing over the transfer tensors  $(\beta_t)_{t \in I(T)}$  associated with the Hierarchical Tucker representation of  $\alpha$  (see Section 2.2.3). Let  $\alpha = F(\{\beta^t\}_{t \in I(T)})$  be a parametrization of  $\alpha$ , where F is a multilinear map, and let  $F_t$  be the partial application of F associated with the transfer tensor  $\beta^t$ ,  $t \in I(T)$ , such that  $F_t(\beta^t) = F(\{\beta^t\}_{t \in I(T)})$ . For a given  $t \in I(T)$ , the minimization on  $\beta^t$  is equivalent to solving a linear system

$$N^t \beta^t = S^t,$$

where  $N^t$  and  $S^t$  are defined such that for all tensors  $\beta^t$  and  $\delta\beta^t$ ,

$$\langle N^t \beta^t, \delta \beta^t \rangle = \sum_{i \in \mathcal{I}_r} \sum_{j \in \mathcal{I}_r} \langle Q_i, Q_j \rangle_\star F_t(\beta^t)_i F_t(\delta \beta^t)_j, \\ \langle S^t, \delta \beta^t \rangle = \sum_{j \in \mathcal{I}_r} \langle A^{-1}, Q_j \rangle_\star F_t(\delta \beta^t)_j.$$

For the practical computation of  $N^t$  and  $S^t$ , we rely on evaluations of the inner product that exploits the hierarchical tensor structure (see [28] for technical details). When  $N^t$  is ill-conditioned, we rather define  $\beta^t$  such that

$$\beta^t \in \arg\min_{\hat{\beta}^t} \left\| N^t \hat{\beta}^t - S^t \right\|.$$

The algorithm for the construction of  $P_r$  is summarized in Algorithm 1.

Algorithm 1: Projection-based algorithm for low-rank approximate inverse construction

Data:  $A \in \mathcal{L}(\mathcal{V}), R \in \mathbb{N}^*, P_0$ Result:  $P_R \in \mathcal{L}(\mathcal{V})$ for  $\mu = 1, ..., d$  do  $\mid \mathcal{U}_0^\mu = 0$ ; end for r = 1, ..., R do  $\mid Compute W_r = \bigotimes_{\mu} W_r^\mu$  by solving  $\min_{W \in \mathcal{C}_1(\mathcal{W})} ||A^{-1} - P_{r-1} - W||_{\star}$ ; for  $\mu = 1, ..., d$  do  $\mid \mathcal{U}_r^\mu = \mathcal{U}_{r-1}^\mu + \operatorname{span}\{W_r^\mu\}$ ; end  $\mathcal{U}_r = \bigotimes_{\mu} \mathcal{U}_r^\mu$ ; Compute  $P_r$  by solving  $\min_{P \in \mathcal{M}} ||A^{-1} - P||_{\star}$  with  $\mathcal{M} = \mathcal{U}_r$  or  $\mathcal{M} = \mathcal{H}_r^T(\mathcal{U}_r)$ ; end return  $P_R$ ;

## 5 Numerical examples

In this section, we apply the proposed Algorithm 1 for the construction of low-rank approximations  $P_r$  of the inverse of operators arising from discretizations of (stochastic) partial differential equations. This algorithm is denoted ALG-P. It is compared with a pure greedy rank-one algorithm for which approximations  $P_r$  are defined by  $P_r = P_{r-1} + W_r$ , where the  $W_r$  are successive rank-one corrections obtained by solving (16), and  $P_r - P_0$  is a tensor with canonical rank r. This algorithm is denoted by ALG-G. For the manipulation of hierarchical Tucker format, we have used the MATLAB<sup>®</sup> toolbox presented in [29].

#### 5.1 Poisson equation

#### 5.1.1 Description of the problem

We consider the Poisson equation defined on the *d*-dimensional domain  $\Omega = \omega^d \subset \mathbb{R}^d$ , with  $\omega = (0, 1)$ , whose solution v(x),  $x = (x_1, \ldots, x_d) \in \Omega$ , satisfies

$$-\sum_{\nu=1}^{d} \frac{\partial^2 v}{\partial x_{\nu}^2} = 1 \quad \text{on} \quad \Omega \quad \text{and} \quad v = 0 \quad \text{on} \quad \partial \Omega.$$

An approximation u of the weak solution  $v \in H_0^1(\Omega) = \bigotimes_{\mu=1}^d H_0^1(\omega)$  is obtained through Galerkin projection in the finite element space  $\mathcal{V} = \bigotimes_{\mu=1}^d \mathcal{V}^{\mu} \subset H_0^1(\Omega)$ , where the  $\mathcal{V}^{\mu} \subset H_0^1(\omega)$  are unidimensional linear finite element spaces. We let  $\mathcal{V}^{\mu} = \operatorname{span}\{\varphi_i; 1 \leq i \leq n\}$ , where  $(\varphi_i)_{1 \leq i \leq n}$  is the linear finite element basis associated with a regular mesh of  $\omega$  composed by n + 1 elements. Therefore,  $\mathcal{V} = \{u = \sum_{i_1=1}^n \dots \sum_{i_d=1}^n \alpha_{i_1\dots i_d} \otimes_{\mu=1}^d \varphi_{i_{\mu}}; \alpha \in \mathbb{R}^n \otimes \dots \otimes \mathbb{R}^n\}$  and the Galerkin approximation  $u \in \mathcal{V}$  is defined by

$$\sum_{\nu=1}^{d} \int_{\Omega} \frac{\partial \delta u}{\partial x_{\nu}} \frac{\partial u}{\partial x_{\nu}} \, dx = \int_{\Omega} \delta u \, dx, \quad \forall \delta u \in \mathcal{V}.$$
<sup>(18)</sup>

By identifying u with the d-order tensor of its coefficients, also denoted  $u \in \mathbb{R}^n \otimes \ldots \otimes \mathbb{R}^n$ , equation (18) is equivalent to the linear system Au = b, with

$$A = \sum_{\nu=1}^{d} \bigotimes_{\mu=1}^{d} (\delta_{\nu\mu} K + (1 - \delta_{\nu\mu})M) , \quad b = \bigotimes_{\mu=1}^{d} c ,$$
  
$$K_{ij} = \int_{\omega} \varphi'_i(x) \varphi'_j(x) \, dx , \quad M_{ij} = \int_{\omega} \varphi_i(x) \, \varphi_j(x) \, dx , \quad c_i = \int_{\omega} \varphi_i(x) dx ,$$

and where  $\delta_{\nu\mu}$  denotes the Kronecker's delta. In the following, we use d = 20 and n = 100.

#### 5.1.2 Numerical results

**Convergence of the sequence of preconditioners** The operator being symmetric positive definite, the approximate inverse is computed with respect to the norm  $\|\cdot\|_* = \|\cdot\|_A$ . For both algorithms ALG-P and ALG-G, we start from  $P_0 = 0$ . In Figure 1 we observe the convergence of the approximate inverse  $P_r$ , by computing the relative error

$$\epsilon(P_r) = \frac{\|I - P_r A\|}{\|I\|} = \frac{\|A^{-1} - P_r\|_{AA^T}}{\|A^{-1}\|_{AA^T}}.$$
(19)

The convergence with r of  $\epsilon(P_r)$  is plotted for both algorithms, with or without imposition of symmetry in the rank-one corrections. For algorithms without imposition of symmetry, we first observe the convergence of  $P_r$  towards  $A^{-1}$ . ALG-P provides a sequence of approximations  $P_r$ which converges very fast compared to the greedy construction. For the same rank r = 10, ALG-P and ALG-G yield errors of  $3.10^{-9}$  and  $3.10^{-2}$  respectively. Algorithms with imposition of symmetry present almost the same convergence, except for a rank greater than 9 corresponding to a very small error less than  $2.10^{-8}$ . Let us emphasize that for computing  $P_r$ , both algorithms require the computation of the same number r of rank-one corrections. For large matrices, these rank-one corrections constitute the most costly step of this algorithm and therefore, for computing  $P_r$ , the two algorithms require almost the same computation times.



Figure 1: Convergence with r of the sequence of approximations  $P_r$  computed with ALG-P (Algorithm 1) or ALG-G (pure greedy algorithm), with or without imposition of symmetry.

**Preconditioned iterative solver** The operator A being symmetric positive definite, we solve the linear system Au = b using a Preconditioned Conjugate Gradient (PCG) with low-rank tensor compressions of the iterates in hierarchical Tucker format (see the algorithm in [27]). Here, we use approximations of the iterates in the hierarchical Tucker subset  $\mathcal{H}_{15}^T(\mathcal{V})$  associated with a balanced tree T (same rank 15 at each node of the tree). We analyze the convergence of the PCG using symmetric preconditioners  $P_r$  constructed with ALG-P or ALG-G. On Figure 2, we observe that the convergence rate of the PCG strongly depends on the quality of the preconditioner. We first note that when using a preconditioner  $P_r$  constructed with a pure greedy algorithm, the convergence of the PCG is not improved when increasing the rank r of the preconditioner. However, when using ALG-P, we can see that the convergence rate rapidly increases with the rank r. Moreover, we observe that the relative residual norm stagnates at a certain precision. This precision depends on two factors: the low-rank subset chosen for the approximation of iterates (here fixed at  $\mathcal{H}_{15}^T(\mathcal{V})$ ) and the quality of the preconditioner. Figure 2 illustrates the strong influence of the preconditioner on the resulting precision, and the superiority of the proposed algorithm over the pure greedy construction. In particular, we observe a difference of 2 (resp. 7) orders of magnitude between rank-5 (resp. rank-10) preconditioners constructed by ALG-G and ALG-P.



Figure 2: Convergence of the Preconditioned Conjugate Gradient using approximate iterates in  $\mathcal{H}_{15}^T(\mathcal{V})$ , and using preconditioners  $\hat{P}_r$  (resp.  $P_r$ ) constructed using ALG-P (resp. ALG-G) with different ranks  $r \in \{1, 5, 10\}$ .

#### 5.2 Stochastic elliptic problem

#### 5.2.1 Description of the problem

We consider the stochastic partial differential equation defined on a 2-dimensional domain  $\Omega = (0,1)^2$ ,

$$-\kappa \Delta v + \eta v = f$$
 on  $\Omega$ ,  $v = 0$  on  $\partial \Omega$ ,

where  $\kappa$  and  $\eta$  are independent random variables with uniform law over the intervals (1, 10) and (200, 1000) respectively. f is such that f(x) = 1 if  $x \in [0.6, 0.8] \times [0.6, 0.8]$  and f(x) = 0 otherwise.  $\kappa$  (resp.  $\eta$ ) is expressed as a linear function  $\kappa(\xi_1)$  (resp.  $\eta(\xi_2)$  of a random variable  $\xi_1$  (resp.  $\xi_2$ ) with uniform law on the interval  $\Xi^1 = (-1, 1)$  (resp.  $\Xi^2$ ), and the solution is expressed under the form  $v(x, \xi_1, \xi_2), x \in \Omega$ , with  $v : \Omega \times \Xi^1 \times \Xi^2 \to \mathbb{R}$ . A Galerkin approximation u of the weak solution  $v \in H_0^1(\Omega) \otimes L^2(\Xi^1) \otimes L^2(\Xi^2)$  is obtained though Galerkin projection in a finite dimensional space  $\mathcal{V} = \mathcal{V}^1 \otimes \mathcal{V}^2 \otimes \mathcal{V}^3$ , where  $\mathcal{V}^1 = \operatorname{span}\{\varphi_i; 1 \le i \le n\} \subset H_0^1(\Omega)$  is a finite element space associated with a regular cartesian mesh of  $\Omega$ , and where  $\mathcal{V}^2 \subset L^2(\Xi^1)$  and  $\mathcal{V}^3 \subset L^2(\Xi^2)$  are polynomial spaces of degree p-1. We denote by  $\{\varphi_i, 1 \le i \le n\}$  the finite element basis of  $\mathcal{V}^1$ . For  $\mathcal{V}^2$  and  $\mathcal{V}^3$ , we introduce a basis  $\{\psi_i; 1 \le i \le p\}$  where  $\psi_{i+1}$  denotes the Legendre polynomial of degree *i*. Therefore,  $\mathcal{V} = \{u = \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{k=1}^{p} \alpha_{ijk} \varphi_i \otimes \psi_j \otimes \psi_k; \alpha \in \mathbb{R}^{n \times p \times p}\}$  and the Galerkin approximation  $u \in \mathcal{V}$  is defined by

$$\int_{\Omega\times\Xi^1\times\Xi^2} (\kappa(y_1)\nabla\delta v \cdot \nabla v + \eta(y_2)\delta v \ v) \ dxdy_1dy_2 = \int_{\Omega\times\Xi^1\times\Xi^2} \delta v \ f(x) \ dxdy_1dy_2 \tag{20}$$

for all  $\delta v \in \mathcal{V}$ . By identifying u with the 3-order tensor of its coefficients, also denoted  $u \in \mathbb{R}^n \otimes \mathbb{R}^p \otimes \mathbb{R}^p$ , equation (20) is equivalent to a linear system Au = b, where A is a rank-2 operator and b is a rank-one tensor. In the following numerical experiments, we take  $n = 20^2$  and p = 10.

#### 5.2.2 Numerical results

**Convergence of the sequence of preconditioners** We construct sequences of low-rank preconditioner  $P_r$  using either ALG-P (Algorithm 1) or ALG-G (pure greedy algorithm), with a norm  $\|\cdot\|_{\star} = \|\cdot\|_A$ . We impose sparsity only along dimension 1. More precisely, during the computation of a rank-one correction  $W_r = W_r^1 \otimes W_r^2 \otimes W_r^3$ , we search for a sparse approximation  $W_r^1$  using the adaptive algorithm presented in Section 3.5.2, with a number of nonzero components limited to a certain percentage, denoted  $\gamma$ , of the total number of components  $n^2$ . The convergence with r of the different preconditioners is illustrated in Figure 3, where the error estimator  $\epsilon(P_r)$  is defined by equation (19). We observe that all algorithms seem to converge toward the inverse of the operator A. As we could have expected, the higher  $\gamma$ , the better the approximation is. Compared to ALG-G, ALG-P significantly improves the quality of the approximation for a low additional cost. For  $\gamma = 30\%$ , ALG-P provides for r = 4 a better approximation than the approximation provided by ALG-G for r = 10.



Figure 3: Convergence with r of the sequence of approximations  $P_r$  computed with ALG-P (Algorithm 1) or ALG-G (pure greedy rank-one algorithm). Sparsity along dimension 1 is imposed with a maximum percentage  $\gamma$  of nonzero components, for  $\gamma = 10, 30, 100\%$ .

**Preconditioned iterative solver** Although the operator A is symmetric positive definite, the resulting preconditioner with imposed sparsity is non symmetric. For the solution of the linear system, we therefore use a preconditioned GMRES (without restart) with low-rank approximations of the iterates (see the algorithm in [3]). Approximations of the iterates are here computed in the subset  $\mathcal{T}_m(\mathcal{V})$  of rank-(m, m, m) Tucker tensors using the Higher Order Orthogonal Iterations (HOOI) algorithm [9].

In the following, we consider preconditioners with imposed sparsity with  $\gamma = 30\%$ . Preconditioners constructed with ALG-P and ALG-G are compared with mean-based preconditioner  $P_E$  which is classically used in the context of stochastic Galerkin methods.  $P_E$  is the sparse

approximate inverse of the rank-one operator associated with a mean-value of the parameters:  $(\kappa, \eta) = (5.5, 600)$ . A reference solution  $u_{\text{ref}}$  is computed with the projection algorithm from [17], which yields a relative residual of 2.40  $10^{-15}$  after 20 iterations. In Figure 4, we illustrate the convergence of the preconditioned GMRES for different preconditioners by plotting the relative error  $\varepsilon(u^{(k)})$  between the k-th iterate  $u^{(k)}$  of GMRES and the reference solution  $u_{\text{ref}}$ , defined by

$$\varepsilon(u^{(k)}) = \frac{\left\|u^{(k)} - u_{\mathrm{ref}}\right\|}{\left\|u_{\mathrm{ref}}\right\|}.$$
(21)



Figure 4: Convergence of the Preconditioned GMRES using approximate iterates in  $\mathcal{T}_5(\mathcal{V})$  (top) or  $\mathcal{T}_{10}(\mathcal{V})$  (bottom), and using preconditioners  $\hat{P}_r$  (resp.  $P_r$ ) constructed using ALG-P (resp. ALG-G) with different ranks  $r \in \{1, 5, 10\}$ . Comparison with the mean based preconditioner  $P_E$ .

We observe that all the rank-one preconditioners give similar convergences, and that ALG-P greatly improves the convergence rate of the preconditioned GMRES algorithm. We observe a stagnation of the relative error at a certain precision. This precision depends on the tensor subset in which the iterates are approximated (here  $\mathcal{T}_{10}(\mathcal{V})$  or  $\mathcal{T}_5(\mathcal{V})$ ) and also on the conditioning of the operator. The final precision can first be improved by introducing larger tensor subsets for the approximation of iterates (compare the precisions obtained using  $\mathcal{T}_{10}(\mathcal{V})$  or  $\mathcal{T}_5(\mathcal{V})$ ). This was already observed in [27, 3]. Also, the final precision can be improved by using a better preconditioner. Figures 4 (top and bottom) illustrate that the relative error for an approximation in  $\mathcal{T}_5(\mathcal{V})$  and a preconditioner  $\hat{P}_{10}$  obtained with ALG-P is 1.4 10<sup>-4</sup>, while the relative error for an approximation in  $\mathcal{T}_{10}(\mathcal{V})$  and a preconditioner  $P_1$  is 2.3  $10^{-4}$ . Concerning the case where the iterates are approximated in  $\mathcal{T}_{10}(\mathcal{V})$  (Figure 4 bottom), we observe that the final relative error slightly increases with the rank r of the preconditioner  $P_r$  constructed by ALG-G. This reflects the fact that when using ALG-G, increasing r only slightly improves the quality of the preconditioner and may result in a deterioration of the final precision measured in solution norm. However, the convergence rate of GMRES clearly increases with r. In practice, when a preconditioner P is available, the error can be estimated by computing the norm of the preconditioned relative residual defined by

$$\widetilde{\varepsilon}(u^{(k)};P) = \frac{\left\|P(b - Au^{(k)})\right\|}{\left\|Pb\right\|}.$$

For good preconditioners,  $\tilde{\varepsilon}(u^{(k)}; P)$  may be a good estimate of the relative error  $\varepsilon(u^{(k)})$  in solution norm. This is illustrated on Figure 5 where we can see that  $\tilde{\varepsilon}(u^{(k)}; P)$  gives almost the same error as  $\varepsilon(u^{(k)})$  when the preconditioner P is a good approximation of  $A^{-1}$  (e.g.  $P = P_5, P_{10}, \hat{P}_5, \hat{P}_{10}$ ).

Influence of sparsity We consider the preconditioner  $\hat{P}_5$  obtained with ALG-P. The convergence of the preconditioned GMRES solver using approximations of iterates in  $\mathcal{T}_{10}(\mathcal{V})$  for different levels  $\gamma$  of sparsity is plotted in Figure 6. We observe that the preconditioning greatly improves the convergence rate of GMRES and also the accuracy of the resulting approximation. As we could have expected, increasing  $\gamma$  improves the preconditioner and therefore improves the convergence rate and the quality of the resulting approximation. When  $\gamma = 100\%$ , that means without imposed sparsity, the algorithm converges very fast and the error  $\varepsilon(u^{(k)})$  stagnates at a very low value of 3  $10^{-9}$  after only 4 iterations. When  $\gamma = 2\%$ , 10% or 30%, we observe that the error  $\varepsilon(u^{(k)})$  stagnates at about the same value 3  $10^{-6}$ , which is greater than for  $\gamma = 100\%$  but also significantly lower than the final error of 1.7  $10^{-2}$  obtained when no preconditioner is used.



Figure 5: Convergence of the Preconditioned GMRES using approximate iterates in  $\mathcal{T}_5(\mathcal{V})$  for different error estimators: relative residual norm (top), relative error in solution norm (middle) and preconditioned relative residual norm (bottom). Use of preconditioners  $\hat{P}_r$  (resp.  $P_r$ ) constructed with ALG-P (resp. ALG-G) with different ranks  $r \in \{1, 5, 10\}$ . Comparison with the mean based preconditioner  $P_E$ .



Figure 6: Convergence of Preconditioned GMRES using approximate iterates in  $\mathcal{T}_{10}(\mathcal{V})$  and using preconditioner  $\hat{P}_5$  constructed using ALG-P with different sparsity levels:  $\gamma = 2, 10, 30, 100\%$ .

## 6 Conclusion

An algorithm has been proposed for the progressive construction of low-rank approximations of the inverse of an operator given in low-rank tensor format. This construction is based on an updated greedy algorithm which consists in constructing a sequence of tensor subspaces from successive rank-one corrections and in computing projections (or approximate projections) in these tensor subspaces, thus resulting in approximations in low-rank Tucker (or Hierarchical Tucker) format. Some desired properties can be imposed on the approximate inverse during the correction step, such as symmetry (requiring the solution of Sylvester equations) or sparsity. For the latter case, the algorithm relies on a straightforward adaptation of the SParse Approximate Inverse method with adaptive selection of the pattern. Compared to a direct approximation in low-rank tensor subsets, the updated greedy algorithm has the advantages of being adaptive and of allowing the reduction of the complexity of the construction. Also, the projection step significantly improves the quality of preconditioners which may be obtained with pure greedy rank-one algorithms. Numerical examples have illustrated the ability of the algorithm to provide good preconditioners for linear systems of equations with a significant improvement of the convergence properties of iterative solvers. The final precision which can be obtained in fixed low-rank tensor subsets is enhanced as well.

Further investigations are needed in order to measure the quality of the approximate inverse as a preconditioner of a linear system of equations. This measure could provide pertinent stopping criteria for the updated greedy algorithm, with a necessary balance between the quality of the preconditioner and the computational complexity (complexity of its construction and of algorithms for solving the preconditioned system).

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