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On low-rank approximability of solutions to high-dimensional operator equations and eigenvalue problems

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Abstract

Low-rank tensor approximation techniques attempt to mitigate the overwhelming complexity of linear algebra tasks arising from high-dimensional applications. In this work, we study the low-rank approximability of solutions to linear systems and eigenvalue problems on Hilbert spaces. Although this question is central to the success of all existing solvers based on low-rank tensor techniques, very few of the results available so far allow to draw meaningful conclusions for higher dimensions. In this work, we develop a constructive framework to study low-rank approximability. One major assumption is that the involved linear operator admits a low-rank representation with respect to the chosen tensor format, a property that is known to hold in a number of applications. Simple conditions, which are shown to hold for a fairly general problem class, guarantee that our derived low-rank truncation error estimates do not deteriorate as the dimensionality increases.

Keywords: Low-rank tensor approximation; High-dimensional equations; Singular value decay; Richardson iteration

Mathematics Subject Classification: 15A18; 15A69; 41A25; 41A46; 41A63; 65J10

1 Introduction

The past few years have seen a growing activity in applying low-rank tensor techniques to the approximate solution of high-dimensional problems, see, e.g., [11, 13] for survey. The success of these techniques crucially depends on the ability to approximate the object of interest by a tensor of low rank with respect to the chosen tensor format. Although this property has been frequently confirmed in practice, there is little theoretical insight into this matter so far.

An important special case of the problems considered in this work are matrix equations of the form $\mathbf{A}(U) = B$ for a linear operator $\mathbf{A} : \mathbb{R}^{M\times N} \to \mathbb{R}^{M\times N}$. Clearly, any such operator can be written in the form

$$\mathbf{A}(U) = A_1^{(1)} U A_1^{(2)} + A_2^{(1)} U A_2^{(2)} + \cdots + A_{r_\mathbf{A}}^{(1)} U A_{r_\mathbf{A}}^{(2)}, \qquad A_i^{(1)} \in \mathbb{R}^{M\times M}, \quad A_i^{(2)} \in \mathbb{R}^{N\times N}$$

for some $r_\mathbf{A} \le MN$. For $r_\mathbf{A} = 1$ and invertible matrices $A_1^{(1)}$, $A_1^{(2)}$ the rank of the solution U equals the rank of B. This property does not hold for $r_\mathbf{A} \ge 2$ and one then considers the question of

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low-rank approximability of U, that is, the decay of its singular values. Particular attention has been paid to the case of a Lyapunov matrix equation

$$AU + UA^T = B$$

for a matrix B of low rank, which plays an important role in control and model reduction, see, e.g., [6]. A number of works [1, 4, 9, 10, 12, 25, 26] have been devoted to studying low-rank approximability for this problem. In particular, it has be shown that the singular values of U decay exponentially when A is symmetric positive definite. All existing proof techniques implicitly rely on the fact that the two operators $U \mapsto AU$ and $U \mapsto UA^T$ commute. In particular, this allows for the simultaneous diagonalization of both operators, which greatly simplifies the approximation problem. When this commutativity property is lost, these techniques fail. For example, only partial results [5, 21] are available so far for the innocently looking modification

$$AU + UA^T + CUC^T = B$$

for general matrix C, which plays a role in bilinear and stochastic control. This indicates that we cannot expect to obtain exponential singular value decay for such generalizations.

In general, we consider linear systems and eigenvalue problems of the form

$$\mathbf{Au} = \mathbf{b}, \qquad \mathbf{Au} = \lambda \mathbf{u}, \tag{1}$$

where $\mathbf{A}$ is a self-adjoint positive definite and bounded linear operator on a tensor product $H_1 \otimes \cdots \otimes H_d$ of Hilbert spaces H_μ, $\mu = 1, \ldots, d$. We will study the low-rank approximability of the solution $\mathbf{u} \in H_1 \otimes \cdots \otimes H_d$ in certain tensor network formats, such as the tensor train format [22] (matrix product states [24]) and the hierarchical Tucker format [14] (tensor tree networks [28]). For these formats, the low-rank approximability is closely tied to the singular value decays of certain bilinear unfoldings associated with the tensor [13]. This plays an important role in the study of quantum many-body systems [27], where these decays are reflected in bounds on the entanglement entropy [8]. For linear lattice models, rigorous bounds by Hastings [15] imply a low-rank approximability that does *not* deteriorate as the order d increases. In the special case of frustration-free systems, similar results [2] can be derived via a simplified construction that only takes the algebraic properties of the involved operators into account.

The purpose of this work is to propose a general framework for obtaining singular value decay estimates for the solutions of (1). Following the basic idea of [2], our results are based on controlling the rank growth of a fixed-point iteration. This approach is constructive and only exploits the tensor product structure of the involved operators. The assumed structure features quite frequently in applications, for example in Schrödinger type eigenvalue problems [17, 20], quantum many-body systems with local interactions [27], the chemical master equation for simulating biochemical reaction networks [16], and Markov models for queuing networks [18]. Under certain conditions, the derived estimates do not deteriorate with increasing d. Our construction shares similarities with recent results by Bachmayr and Dahmen [3], who use the method of steepest descent to design a nearly optimal solver for linear systems. In contrast to our work, these results *assume* the low-rank approximability of the solution a priori.

Our results state algebraic approximation rates with respect to increasing ranks. An exponential approximation rate can only be obtained under certain commutativity assumptions, similar to the Lyapunov equation discussed above. One of the very few results in this direction is the approximation of the solution to the d-dimensional Poisson equation by means of exponential sums [9, 13].

The rest of this paper is organized as follows. In Section 2, we provide a general framework for assessing the interplay between rank growth and convergence rate of fixed point iterations on tensor products of Hilbert spaces. Section 3 specializes this framework to the method of steepest descent applied to linear systems with tensor product structure, resulting in singular value decay estimates for the solution. In a similar manner, Section 4 covers symmetric eigenvalue problems.

2 Approximation by fixed-point iterations with finite rank growth

In this section, we develop our general framework for low-rank tensor approximation by first considering the case $d = 2$ and then extending these results to tensors of arbitrary order d.

2.1 Bilinear approximation

Let H_1, H_2 be two Hilbert spaces (either both real or both complex), and consider the tensor product $\mathbf{H} = H_1 \otimes H_2$ with the induced inner product $\langle u_1 \otimes v_1, u_2 \otimes v_2 \rangle_{\mathbf{H}} = \langle u_1, v_1 \rangle_{H_1} \cdot \langle u_2, v_2 \rangle_{H_2}$. Note that $\mathbf{H}$ is isomorphic to $HS(H_1, H_2)$, the space of Hilbert-Schmidt operators from H_2 to H_1. Every tensor $\mathbf{u} \in \mathbf{H}$ admits a *singular value decomposition* (SVD)

$$\mathbf{u} = \sum_{k=1}^{\infty} \sigma_k u_k \otimes v_k, \tag{2}$$

with $u_1, u_2, \dots$ and $v_1, v_2, \dots$ forming complete orthonormal systems in H_1 and H_2, respectively, and *singular values* $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$. The smallest r for which $\sigma_{r+1} = 0$ is called the rank of $\mathbf{u}$. If there is no such r, the rank of $\mathbf{u}$ is ∞.

We denote by

$$\tau_r(\mathbf{u}) = \inf_{\substack{\tilde{u}_1, \dots, \tilde{u}_r \in H_1 \\ \tilde{v}_1, \dots, \tilde{v}_r \in H_2}} \left\| \mathbf{u} - \sum_{k=1}^{r} \tilde{u}_k \otimes \tilde{v}_k \right\|_{\mathbf{H}}$$

the error for the best bilinear approximation of rank at most r. It is well known that the infimum is achieved by the sum of the first r terms in the singular value decomposition, and

$$\tau_r(\mathbf{u}) = \min_{\operatorname{rank}(\mathbf{v}) \leq r} \|\mathbf{u} - \mathbf{v}\|_{\mathbf{H}} = \left(\sum_{k=r+1}^{\infty} \sigma_k^2 \right)^{1/2}.$$

In the sequel we will be concerned with the case that $\mathbf{u}$ is implicitly given, e.g., as the solution of an optimization problem that represents a linear operator equation or eigenvalue problem. The basis of our framework is to approach $\mathbf{u}$ by a fixed-point iteration

$$\mathbf{u}_{n+1} = \Phi(\mathbf{u}_n) \tag{3}$$

which has a guaranteed convergence rate, but increases the ranks of the iterates at most by a constant factor in every step. Examples for (3) relevant for linear systems are gradient descent methods, like the Richardson iteration that will be used later on. However, other fixed-point iterations are imaginable wherefore we first keep the setting general. We need the following properties.

(i) *Contraction:* There exists $0 < q < 1$ and $c > 0$ such that

$$\|\mathbf{u}_{n+1} - \mathbf{u}\|_{\mathbf{H}} \leq c q^{n+1} \|\mathbf{u}_0 - \mathbf{u}\|_{\mathbf{H}} \quad \text{for all } n. \tag{A1}$$

(ii) *Finite rank growth:* There exists $R > 1$ such that

$$\operatorname{rank}(\mathbf{u}_{n+1}) \leq R \cdot \operatorname{rank}(\mathbf{u}_n) \quad \text{for all } n. \tag{A2}$$

The missing ingredient is that the starting point $\mathbf{u}_0$ should have known finite rank. In fact, we will assume that $\operatorname{rank}(\mathbf{u}_0) \leq 1$. The limit point (as well as the other properties) of the iteration may depend on the choice of $\mathbf{u}_0$ (this will become particularly visible for the case of eigenvalue problems in Section 4). We therefore consider a set

$$\mathcal{D} \subseteq \{\mathbf{u}_0 : \text{the sequence } (\mathbf{u}_n) \text{ generated from } \mathbf{u}_0 \text{ by (3) satisfies (A1) and (A2)}\}, \tag{4}$$

and assume

(iii) *Rank-one starting point:* Properties (A1) and (A2) can be satisfied using a starting point in $\mathcal{D}$ with rank at most one, that is,

$$\mathcal{D} \cap \{\mathbf{u}_0 \in \mathbf{H} : \operatorname{rank}(\mathbf{u}_0) \leq 1\} \neq \emptyset. \tag{A0}$$

Given (A0), one can define the quantity

$$\pi_1(\mathbf{u}) = \inf_{\substack{\mathbf{v} \in \mathcal{D} \\ \operatorname{rank}(\mathbf{v}) \leq 1}} \|\mathbf{v} - \mathbf{u}\|_{\mathbf{H}},$$

and derive the main result of this section.

Theorem 1. *The existence of a map* Φ *on* $\mathbf{H}$ *satisfying* (A0) *implies*

$$\tau_r(\mathbf{u}) \leq c\pi_1(\mathbf{u}) \sqrt{\left(1 - \frac{(1-q^2)(r - R^{\lfloor \log_R r \rfloor})}{(R-1)R^{\lfloor \log_R r \rfloor}}\right)} q^{\lfloor \log_R r \rfloor}. \tag{5}$$

Simplified bounds are given by

$$\tau_r(\mathbf{u}) \leq c\pi_1(\mathbf{u}) q^{\lfloor \log_R r \rfloor} \leq c\pi_1(\mathbf{u}) q^{(\log_R r)-1} = c\pi_1(\mathbf{u}) q^{-1} \left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R}\right|}. \tag{6}$$

Proof. For brevity, we write τ_r instead of $\tau_r(\mathbf{u})$. By (A0), there is a starting point $\mathbf{u}_0 \in \mathcal{D}$ of rank at most one such that the sequence $(\mathbf{u}_n)$ formed by (3) satisfies (A1) and (A2). Consequently, $\operatorname{rank}(\mathbf{u}_n) \leq R^n$ and

$$\tau_{R^n} \leq \|\mathbf{u}_n - \mathbf{u}\|_{\mathbf{H}} \leq cq^n \|\mathbf{u}_n - \mathbf{u}_0\|_{\mathbf{H}}.$$

As this holds for all admissible $\mathbf{u}_0$, we may pass to the infimum:

$$\tau_{R^n} \leq c\pi_1(\mathbf{u}) q^n. \tag{7}$$

Since the sequence (σ_k) is decreasing, we have for every $0 \leq s < R^{n+1} - R^n$ that

$$\sum_{k=R^n+1}^{R^n+s} \sigma_k^2 \geq \frac{s}{R^{n+1} - R^n} \sum_{k=R^n+1}^{R^{n+1}} \sigma_k^2 = \frac{s}{(R-1)R^n} (\tau_{R^n}^2 - \tau_{R^{n+1}}^2).$$

Hence, using (7), we obtain for $r = R^n + s$ the estimate

$$\tau_r^2 = \tau_{R^n}^2 - \sum_{k=R^n+1}^{R^n+s} \sigma_k^2 \le \tau_{R^n}^2 - \frac{s}{(R-1)R^n}(\tau_{R^n}^2 - \tau_{R^{n+1}}^2)$$
$$\le c^2\pi_1(\mathbf{u})^2 \left(1 - \frac{(1-q^2)s}{(R-1)R^n}\right) q^{2n},$$

as asserted by (5). The simplified bound (6) follows from the observation that the term under the square root in (5) is bounded by one. □

By general results for ordered sequences [7], a decay rate for the tail $\tau_r(\mathbf{u})$ yields a decay rate for the singular values themselves. For instance, using (6), we obtain

$$\sigma_r^2 \le \frac{\sum_{k=\lfloor r/2\rfloor+1}^{r} \sigma_k^2}{r - \lfloor r/2\rfloor} \le \frac{\tau_{\lfloor r/2\rfloor}^2(\mathbf{u})}{\lfloor r/2\rfloor} \le c\pi_1(\mathbf{u}) q^{-2} \left(\frac{1}{\lfloor r/2\rfloor}\right)^{2\left|\frac{\ln q}{\ln R}\right|} \le c\pi_1(\mathbf{u}) q^{-2} \left(\frac{2}{r-1}\right)^{2\left|\frac{\ln q}{\ln R}\right|}. \quad (8)$$

One consequence of (8) is that the von Neumann entropy of the squared singular values,

$$S(\mathbf{u}) = \sum_{k=1}^{\infty} \sigma_k^2 \log(\sigma_k^2),$$

remains finite under the conditions of Theorem 1, that is, if a fixed-point iteration with the property (A0) exists. This is non-trivial since the mere membership of $\mathbf{u} \in H_1 \otimes H_2$ only implies the series $\sum_{k=1}^{\infty} \sigma_k^2$ to converge. Explicit bounds on the von Neumann entropy $S(\mathbf{u})$ are of interest in many applications, for instance in quantum particle models where it represents the *entanglement entropy* of ground states [2, 8, 15].

2.2 Multilinear approximation

We now consider $d \ge 2$ Hilbert spaces $H_1, H_2, \ldots, H_d$ (either all real or all complex). For each subset $t \subseteq \{1, 2, \ldots, d\}$ of indices with $0 < |t| < d$, we have the following isomorphism between the tensor product Hilbert space

$$\mathbf{H} = H_1 \otimes H_2 \otimes \cdots \otimes H_d$$

and Hilbert-Schmidt operators:

$$\mathbf{H} \cong HS\left(\bigotimes_{\mu \in t} H_\mu, \bigotimes_{\nu \notin t} H_\nu\right), \quad (9)$$

see, e.g., [13]. In the finite-dimensional case, this simply amounts to reshaping the tensor into a matrix, with the indices corresponding to t merged into the row indices.

The isomorphism (9) allows us to introduce the *t-rank* of $\mathbf{u} \in \mathbf{H}$, denoted by $\mathrm{rank}^{(t)}(\mathbf{u})$, as the rank of the associated Hilbert-Schmidt operator. Correspondingly, the sequence of singular values $(\sigma_k^{(t)})$, and the best bilinear approximation errors

$$\tau_r^{(t)}(\mathbf{u}) = \min_{\mathrm{rank}^{(t)}(\mathbf{v}) \le r} \|\mathbf{u} - \mathbf{v}\|_{\mathbf{H}} = \left(\sum_{k=r+1}^{\infty} (\sigma_k^{(t)})^2\right)^{1/2}$$

can be defined.

Theorem 1 implies for fixed t that

$$\tau_r^{(t)}(\mathbf{u}) \leq c\pi_1^{(t)}(\mathbf{u})q^{-1}\left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R^{(t)}}\right|} \tag{10}$$

under slightly modified assumptions. In particular, the property (A2) is replaced by

$$\operatorname{rank}^{(t)}(\mathbf{u}_{n+1}) \leq R^{(t)} \cdot \operatorname{rank}^{(t)}(\mathbf{u}_n)$$

for some $R^{(t)} > 0$. The other properties remain the same. In principle, the constants q and c involved in (A1) could also depend on t but, for simplicity, we omit this dependence. With $\mathcal{D}$ defined as in (4), the analogue of the main assumption (A0) is that the quantity

$$\pi_1^{(t)}(\mathbf{u}) = \inf_{\substack{\mathbf{v}\in\mathcal{D} \\ \operatorname{rank}^{(t)}(\mathbf{v})\leq 1}} \|\mathbf{v}-\mathbf{u}\|_{\mathbf{H}} \tag{11}$$

is finite.

Knowing the decay properties of $\tau_r^{(t)}(\mathbf{u})$ for certain choices of t is crucial for understanding the approximability of $\mathbf{u}$ in subspace based low-rank tensor formats. For instance, the tensor train format [22] involves the t-ranks of $t = \{1,2,\dots,\mu\}$ for $\mu = 1,2,\dots,d-1$. For prescribed ranks r_μ, the best approximation error in this format admits the quasi-optimal bound [23, Thm. 2.2]

$$\sqrt{\left(\tau_{r_1}^{\{1\}}(\mathbf{u})\right)^2 + \left(\tau_{r_2}^{\{1,2\}}(\mathbf{u})\right)^2 + \cdots + \left(\tau_{r_{d-1}}^{\{1,\dots,d-1\}}(\mathbf{u})\right)^2}.$$

More specifically, d-independent bounds on the von Neumann entropies of the singular values $(\sigma_k^{(t)})$ for these specific choices of t constitute one-dimensional *area laws* in the theory of quantum spin systems [2, 8, 15].

3 Linear equations with low-rank operators and low-rank data

We now apply the general framework from Section 2 to a linear system

$$\mathbf{A}\mathbf{u} = \mathbf{b}, \tag{12}$$

where $\mathbf{A}$ is a self-adjoint operator on $\mathbf{H}$ with

$$\gamma\|\mathbf{v}\|_{\mathbf{H}}^2 \leq \langle \mathbf{v}, \mathbf{A}\mathbf{v}\rangle_{\mathbf{H}} \leq \Gamma\|\mathbf{v}\|_{\mathbf{H}}^2 \tag{13}$$

for some $0 < \gamma < \Gamma$. In particular, this is the case when all Hilbert space are finite-dimensional and $\mathbf{A}$ is a Hermitian positive definite matrix acting on $\mathbf{H}$.

The solution $\mathbf{u}$ of (12) is a fixed-point of the *Richardson iteration*

$$\mathbf{u}_{n+1} = \Phi(\mathbf{u}_n) := \mathbf{u}_n - \alpha(\mathbf{A}\mathbf{u}_n - \mathbf{b}), \quad \alpha = \frac{2}{\gamma+\Gamma}. \tag{14}$$

It is well-known that the convergence rate is bounded as follows:

$$\|\mathbf{I} - \alpha\mathbf{A}\|_{\mathbf{H}\to\mathbf{H}} \leq \frac{\kappa-1}{\kappa+1} < 1,$$

with the condition number $\kappa = \Gamma/\gamma$. Therefore,

$$\|\mathbf{u}_{n+1} - \mathbf{u}\|_{\mathbf{H}} \leq \left(\frac{\kappa-1}{\kappa+1}\right)^{n+1} \|\mathbf{u}_0 - \mathbf{u}\|_{\mathbf{H}} \tag{15}$$

holds for all $n \geq 0$.

For a fixed choice of $t \subseteq \{1,2,\ldots,d\}$, $0 < |t| < d$, we now assume that the operator and right-hand side admit a low-rank representation with respect to the splitting (9):

$$\mathbf{A} = \sum_{i=1}^{r_{\mathbf{A}}^{(t)}} A_i^{(t)} \otimes A_i^{(t^c)}, \qquad \mathbf{b} = \sum_{j=1}^{r_{\mathbf{b}}^{(t)}} b_j^{(t)} \otimes b_j^{(t^c)}, \tag{16}$$

where $t^c = \{1,2,\ldots,d\} \setminus t$. Note that we can always assume $r_{\mathbf{b}}^{(t)} \leq r_{\mathbf{A}}^{(t)}$ by superposition.

Theorem 2. *Given* (13) *and* (16) *with* $r_{\mathbf{b}}^{(t)} \leq r_{\mathbf{A}}^{(t)}$*, the solution* $\mathbf{u}$ *of* (12) *satisfies*

$$\tau_r^{(t)}(\mathbf{u}) \leq \frac{\|\mathbf{u}\|_{\mathbf{H}}}{q} \left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R^{(t)}}\right|} \tag{17}$$

with $R^{(t)} = r_{\mathbf{A}}^{(t)} + 2$ *and* $q = \frac{\kappa-1}{\kappa+1}$*. If, additionally,* $A_i^{(t)}$ *or* $A_i^{(t^c)}$ *in* (16) *is the identity for some i, then* (17) *holds with* $R^{(t)} = r_{\mathbf{A}}^{(t)} + 1$.

Proof. By expanding all terms, one concludes from (14) and (16) that

$$\operatorname{rank}^{(t)}(\mathbf{u}_{n+1}) \leq \operatorname{rank}^{(t)}(\mathbf{u}_n) + r_{\mathbf{A}}^{(t)} \operatorname{rank}^{(t)}(\mathbf{u}_n) + r_{\mathbf{b}}^{(t)} \leq (r_{\mathbf{A}}^{(t)} + 2) \operatorname{rank}^{(t)}(\mathbf{u}_n). \tag{18}$$

Taking also (15) into account, we see that for any starting point $\mathbf{u}_0 \in \mathbf{H}$ the conditions (A1) and (A2) hold with $q = \frac{\kappa-1}{\kappa+1}$, $c = 1$, and $R^{(t)} = r_{\mathbf{A}}^{(t)} + 2$. Hence, the domain $\mathcal{D}$ considered in (4) can be taken to be $\mathcal{D} = \mathbf{H}$ for this choice of parameters, and therefore (A0) trivially holds. Considering $\mathbf{u}_0 = \mathbf{0}$ yields the estimate $\pi_1^{(t)}(\mathbf{u}) \leq \|\mathbf{u}\|_{\mathbf{H}}$. Consequently, the first part of the theorem is an instance of (10).

To show the second part, we may assume w.l.o.g. that $A_1^{(t)} = I$ in (16). Then we can rewrite

$$\mathbf{u}_n - \alpha \mathbf{A}\mathbf{u}_n = \left(I \otimes (I - \alpha A_1^{(t)}) - \alpha \sum_{i=2}^{r_{\mathbf{A}}^{(t)}} A_i^{(t)} \otimes A_i^{(t^c)} \right) \mathbf{u}_n,$$

so that the rank actually increases at most by a factor of $R^{(t)} = r_{\mathbf{A}}^{(t)} + 1$. □

Example 1. *The following structure occurs frequently in applications of high-dimensional operator equations:*

$$\mathbf{A} = \mathbf{L} + \mathbf{V}, \tag{19}$$

where

$$\mathbf{L} = A_1 \otimes I \otimes \cdots \otimes I + I \otimes A_2 \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes A_d,$$
$$\mathbf{V} = B_1 \otimes C_2 \otimes I \otimes \cdots \otimes I + I \otimes B_2 \otimes C_3 \otimes \cdots \otimes I + I \otimes \cdots \otimes I \otimes B_{d-1} \otimes C_d.$$

Here, the μth term of $\mathbf{L}$ represents the action on the μth variable. For example, a structured discretization of the d-dimensional Laplace operator takes this form. The terms in $\mathbf{V}$ describe interactions between two neighboring variables.

We assume that all involved coefficients A_μ, B_μ, and C_μ are bounded self-adjoint operators satisfying the inequalities

$$\gamma_A \le A_\mu \le \Gamma_A, \quad 0 \le B_\mu \le \Gamma_B, \quad 0 \le C_\mu \le \Gamma_C$$

in the spectral sense, for some constants $\gamma_A, \Gamma_A, \Gamma_B, \Gamma_C > 0$ independent of μ. Then $\mathbf{A}$ is a bounded self-adjoint operator satisfying the inequality (13) *with $\gamma = d\gamma_A$ and $\Gamma = d\Gamma_A + (d-1)\Gamma_B\Gamma_C$. Consequently, the condition number κ determining the contraction rate* (15) *is bounded independently of d.*

On the other hand, it can be shown by an explicit construction [17, 19] that any operator having the algebraic structure (19) *admits a low-rank representation of the form* (16) *with $r_{\mathbf{A}}^{(t)} = 3$ for any $t = \{1, 2, \dots, \mu\}$. In turn, the solution to an operator equation with the structure in* (19) *and low-rank right-hand side $\mathbf{b}$ satisfies the decay estimate* (17) *for any such t, independently of d. As discussed at the end of Section 2, this implies d-independent approximability in the tensor train format. By [20, Ex. 5.2], the same conclusion holds for the hierarchical Tucker format.*

Remark 1. *It is instructive to discuss the special case $\mathbf{V} = 0$ in Example 1, which corresponds to the absence of the neighbor interaction terms B_μ and C_μ. Exploiting the commutativity of the d terms in $\mathbf{L}$, one can show that the iterates $\mathbf{u}_n$ produced by the method of steepest descent* (14) *applied to $\mathbf{A} = \mathbf{L}$ satisfy $\operatorname{rank}^{(t)}(\mathbf{u}_n) \le (n+1)\operatorname{rank}^{(t)}(\mathbf{u}_0)$ for each $t = \{1, 2, \dots, \mu\}$. In this case, our analysis can be improved considerably. The error estimate* (7) *in the proof of Theorem 1 can be replaced by $(\tau_n^{(t)})^2 \lesssim (\frac{\kappa-1}{\kappa+1})^{2n}$. In turn, we obtain exponential singular value decays with respect to all such t. Similar and even stronger results can be obtained by approximating the inverse $\mathbf{L}^{-1}$ of the Laplace-like operator $\mathbf{L}$ by exponential sums [9, 13].*

4 Eigenvalue problems with low-rank operators

As another application of our general framework, we now consider the approximability of an eigenvector $\mathbf{u}$ belonging to the smallest eigenvalue λ_1 of a bounded self-adjoint operator $\mathbf{A} : \mathbf{H} \to \mathbf{H}$. In particular, we have

$$\lambda_1 \|\mathbf{v}\|^2 \le \langle \mathbf{v}, \mathbf{A}\mathbf{v} \rangle_{\mathbf{H}} \le \Gamma \|\mathbf{v}\|_{\mathbf{H}}^2, \tag{20}$$

for some Γ.

In the following, we assume λ_1 to be simple. This implies that the rest of the spectrum is contained in an interval $[\lambda_2, \Gamma]$ with $\lambda_2 > \lambda_1$. The *absolute gap* and the *relative gap* are denoted by

$$\delta = \lambda_2 - \lambda_1, \qquad \Delta = \frac{\delta}{\Gamma - \lambda_1}, \tag{21}$$

respectively. These gaps play a critical role in our estimates.

We now fix $\mathbf{u}$, and denote by $\langle \mathbf{u} \rangle$ the linear span of $\mathbf{u}$. To approximate $\mathbf{u}$, we apply the Richardson iteration to the singular linear system

$$\mathbf{A}_{\lambda_1}\mathbf{u} := (\mathbf{A} - \lambda_1 \mathbf{I})\mathbf{u} = \mathbf{0}, \tag{22}$$

but on the nontrivial invariant subspace $\langle \mathbf{u} \rangle^\perp$. This results in the iteration

$$\mathbf{u}_{n+1} = \Phi(\mathbf{u}_n) := \mathbf{u}_n - \beta \mathbf{A}_{\lambda_1} \mathbf{u}_n = (1+\beta\lambda_1)\mathbf{u}_n - \beta \mathbf{A}\mathbf{u}_n, \quad \beta = \frac{2}{\delta + \Gamma - \lambda_1}, \quad \mathbf{u}_0 \in \mathbf{u} + \langle \mathbf{u} \rangle^\perp. \tag{23}$$

We emphasize that this method assumes the knowledge of the exact λ_1 a priori. It is therefore primarily of theoretical interest, to derive the desired error estimates for the low-rank approximability of the eigenvector $\mathbf{u}$. In turn, these estimates could be used to design a practical method of optimal complexity, in the spirit of [3].

In order to apply Theorem 1, we now verify that the properties (A1) and (A2) are satisfied. We begin with discussing the convergence of (23). By the simplicity of λ_1, the self-adjoint operator $\mathbf{A}_{\lambda_1} = \mathbf{A} - \lambda_1 \mathbf{I}$ has the one-dimensional kernel $\langle \mathbf{u} \rangle$. It is bounded from below and above by δ and $\Gamma - \lambda_1$, respectively, on the invariant subspace $\langle \mathbf{u} \rangle^\perp$, so its condition number on this subspace is $1/\Delta$. This implies that the spectral radius of $\mathbf{I} - \beta \mathbf{A}_{\lambda_1}$ on the invariant subspace $\langle \mathbf{u} \rangle^\perp$ is bounded by $\frac{1-\Delta}{1+\Delta}$. Since $\mathbf{u}_{n+1} - \mathbf{u} = (\mathbf{I} - \beta \mathbf{A}_{\lambda_1})(\mathbf{u}_n - \mathbf{u})$, an induction shows that if $\mathbf{u}_0 - \mathbf{u} \in \langle \mathbf{u} \rangle^\perp$, then $\mathbf{u}_n - \mathbf{u} \in \langle \mathbf{u} \rangle^\perp$ for all n, and

$$\|\mathbf{u}_{n+1} - \mathbf{u}\|_{\mathbf{H}} \le \left(\frac{1-\Delta}{1+\Delta}\right)^{n+1} \|\mathbf{u}_0 - \mathbf{u}\|_{\mathbf{H}} \quad \text{if } \mathbf{u}_0 \in \mathbf{u} + \langle \mathbf{u} \rangle^\perp. \tag{24}$$

In other words, (A1) holds with $q = \frac{1-\Delta}{1+\Delta}$.

As for (A2), similar to (18), the t-ranks of the iteration (23) satisfy

$$\operatorname{rank}^{(t)}(\mathbf{u}_{n+1}) \le (r_{\mathbf{A}}^{(t)} + 1) \operatorname{rank}^{(t)}(\mathbf{u}_n), \tag{25}$$

provided that $\mathbf{A}$ admits a representation of the form (16). Once again, if one of the operators $A_i^{(t)}$ or $A_i^{(t^c)}$ in (16) is the identity, then $r_{\mathbf{A}}^{(t)} + 1$ can be replaced by $r_{\mathbf{A}}^{(t)}$ in (25). In both cases, property (A2) is satisfied.

Assumption (A0). By (24), the set $\mathcal{D}$ defined in (4) takes the form

$$\mathcal{D} = \{\mathbf{v} \in \mathbf{H} : \langle \mathbf{v} - \mathbf{u}, \mathbf{u} \rangle_{\mathbf{H}} = 0\}.$$

To verify the main assumption (A0), we have to show that $\mathcal{D}$ contains a starting point having t-rank at most one. In fact, let $\hat{\mathbf{u}}_0$ be any element with $\operatorname{rank}^{(t)}(\hat{\mathbf{u}}_0) = 1$ that is not orthogonal to $\mathbf{u}$. Then

$$\mathbf{u}_0 = \frac{\|\mathbf{u}\|_{\mathbf{H}}^2}{\langle \mathbf{u}, \hat{\mathbf{u}}_0 \rangle_{\mathbf{H}}} \hat{\mathbf{u}}_0 \in \mathcal{D} \tag{26}$$

with $\operatorname{rank}^{(t)}(\mathbf{u}_0) = 1$. In turn, the quantity $\pi_1^{(t)}(\mathbf{u})$ defined in (11) is finite.

Our findings above allow us to apply Theorem 1 for estimating the t-rank approximation error of the eigenvector $\mathbf{u}$.

Theorem 3. *Given* (16) *and* (20)*, the solution* $\mathbf{u}$ *of* (22) *satisfies*

$$\tau_r^{(t)}(\mathbf{u}) \le \frac{\pi_1^{(t)}(\mathbf{u})}{q} \left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R^{(t)}}\right|}, \tag{27}$$

with $q = \frac{1-\Delta}{1+\Delta}$, $R^{(t)} = r_{\mathbf{A}}^{(t)} + 1$*, and the gaps* δ, Δ *defined in* (21)*. If, additionally,* $A_i^{(t)}$ *or* $A_i^{(t^c)}$ *in* (16) *is the identity for some i, then* (27) *holds with* $R^{(t)} = r_{\mathbf{A}}^{(t)}$.

A notable difference of Theorem 3 to Theorem 2 is that it features the quantity $\pi_1^{(t)}(\mathbf{u})$ in the estimate. This quantity measures the distance between $\mathbf{u}$ and the set of t-rank one tensors within the affine space $\mathbf{u}+\langle\mathbf{u}\rangle^{\perp}$. In this way, the problem of rank-r approximability has been reduced to the problem of rank-one approximability.

4.1 The problem of t-rank one approximability

In this section, we derive upper bounds for the quantity $\pi_1^{(t)}(\mathbf{u})$ defined in (11). Trivially, every starting point $\mathbf{u}_0 \in \mathcal{D}$ of t-rank one yields the upper bound $\|\mathbf{u}_0-\mathbf{u}\|_{\mathbf{H}}$. While this is of interest when considering a specific iteration, more insight would be gained from bounds that depend on δ, Δ, and $r_{\mathbf{A}}^{(t)}$ only. Deriving such bounds is surprisingly difficult and at the heart of related works on the entanglement entropy, see, e.g., [2].

In an infinite-dimensional tensor product space $\mathbf{H}$, the ratio $\pi_1^{(t)}(\mathbf{u})/\|\mathbf{u}\|_{\mathbf{H}}$ may become arbitrarily large for arbitrary $\mathbf{u}\in\mathbf{H}$. Upper bounds are obtained from t-rank one approximations to $\mathbf{u}$ in the $\mathbf{H}$-norm. Specifically, considering (26) with $\|\hat{\mathbf{u}}_0\|_{\mathbf{H}}=1$, we get the estimate

$$\pi_1^{(t)}(\mathbf{u}) \le \|\mathbf{u}_0-\mathbf{u}\|_{\mathbf{H}} \le \|\mathbf{u}_0\|_{\mathbf{H}} = \frac{\|\mathbf{u}\|_{\mathbf{H}}}{\left|\left\langle \frac{\mathbf{u}}{\|\mathbf{u}\|_{\mathbf{H}}}, \hat{\mathbf{u}}_0 \right\rangle_{\mathbf{H}}\right|},$$

where we used that $\mathbf{u}_0-\mathbf{u}$ is orthogonal to $\mathbf{u}$. Thus, the problem is further reduced to providing a lower bound on the overlap of the normalized eigenvector with normalized tensors of t-rank one:

$$\pi_1^{(t)}(\mathbf{u}) \le \frac{\|\mathbf{u}\|_{\mathbf{H}}}{\theta_1^{(t)}(\mathbf{u})}, \tag{28}$$

where

$$\theta_1^{(t)}(\mathbf{u}) := \sup_{\substack{\operatorname{rank}^{(t)}(\hat{\mathbf{u}}_0)=1 \\ \|\hat{\mathbf{u}}_0\|_{\mathbf{H}}=1}} \left\langle \frac{\mathbf{u}}{\|\mathbf{u}\|_{\mathbf{H}}}, \hat{\mathbf{u}}_0 \right\rangle_{\mathbf{H}}. \tag{29}$$

In the case that every H_μ has finite dimension N_μ, $\mu=1,\dots,d$, a generic bound is obtained as follows. The singular value decomposition (2) of the solution with respect to the identification (9) is a finite sum with

$$D^{(t)} = \min\left(\prod_{\mu\in t} N_\mu, \prod_{\nu\notin t} N_\nu\right)$$

mutually orthogonal t-rank one tensors of decreasing norms $\sigma_k^{(t)}$. This implies that the overlap (29) is at least $\sigma_1^{(t)}/\|\mathbf{u}\|_{\mathbf{H}} \ge 1/\sqrt{D^{(t)}}$. By (28), we obtain

$$\pi_1^{(t)}(\mathbf{u}) \le \sqrt{D^{(t)}}\|\mathbf{u}\|_{\mathbf{H}}. \tag{30}$$

This bound is independent of d only when the cardinality of t does not grow, which is the case for the Tucker format [13]. The tensor train and hierarchical Tucker formats, however, require to take large splittings like $t=\{1,\dots,d/2\}$ into consideration. Consequently, the bound (30) grows exponentially with d. In [2], one of the very few results on this question, it has been shown how this growth can be avoided in the case of frustration-free systems. This constitutes a rather limiting assumption. The following result adapts a technique from [2, Lemma III.2], which does not require this assumption but instead assumes a rather strong contraction relative to the rank growth.

Theorem 4. *With the notation introduced in Theorem 3, assume that $q^2R^{(t)} < 1$. Then it holds*

$$\left(\theta_1^{(t)}(\mathbf{u})\right)^2 \geq \frac{1}{2}\left(\frac{1}{R^{(t)}}\right)^{\left\lceil \frac{-\ln 2}{\ln\left(q^2R^{(t)}\right)} \right\rceil}$$

for $\theta_1^{(t)}(\mathbf{u})$ defined in (29)*. Consequently, by* (27) *and* (28)*,*

$$\tau_r^{(t)}(\mathbf{u}) \leq \sqrt{2}(R^{(t)})^{\frac{1}{2}\left\lceil \frac{-\ln 2}{\ln\left(q^2R^{(t)}\right)} \right\rceil} \|\mathbf{u}\|_{\mathbf{H}} \left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R^{(t)}}\right|}.$$

Proof. Without loss of generality, we may assume $\|\mathbf{u}\|_{\mathbf{H}} = 1$. Let P denote the orthogonal projection onto $\langle \mathbf{u} \rangle$. To simplify the notation, we write θ instead of $\theta_1^{(t)}(\mathbf{u})$.

Let $\varepsilon > 0$ and $\hat{\mathbf{u}}_0$ be an normalized rank-one tensor with $\|P\hat{\mathbf{u}}_0\|_{\mathbf{H}} = \langle \mathbf{u}, \hat{\mathbf{u}}_0 \rangle_{\mathbf{H}} \geq \theta - \varepsilon$. We let $\hat{\mathbf{u}}_n$ denote the iterate obtained after n steps of the Richardson method (23) with starting vector $\hat{\mathbf{u}}_0$. Since $\hat{\mathbf{u}}_0 \in P\hat{\mathbf{u}}_0 + \langle \mathbf{u} \rangle^{\perp}$, this rescaled Richardson method converges to $P\hat{\mathbf{u}}_0 \neq 0$ and, by induction,

$$P\hat{\mathbf{u}}_n = P\hat{\mathbf{u}}_0. \tag{31}$$

By (24) and using $\|\hat{\mathbf{u}}_0\|_{\mathbf{H}} = 1$,

$$\|(I-P)\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2 \leq q^{2n}\|(I-P)\hat{\mathbf{u}}_0\|_{\mathbf{H}}^2 = q^{2n}(1 - \|P\hat{\mathbf{u}}_0\|_{\mathbf{H}}^2).$$

Hence,

$$\begin{aligned} \|\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2 &= \|P\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2 + \|(I-P)\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2 = \|P\hat{\mathbf{u}}_0\|_{\mathbf{H}}^2 + \|(I-P)\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2 \\ &\leq \|P\hat{\mathbf{u}}_0\|_{\mathbf{H}}^2 + q^{2n}(1 - \|P\hat{\mathbf{u}}_0\|_{\mathbf{H}}^2) \\ &\leq \theta^2 + q^{2n}(1-(\theta-\varepsilon)^2), \end{aligned} \tag{32}$$

where we used that $\|P\hat{\mathbf{u}}_0\|_{\mathbf{H}} \leq \theta$ by definition (29) of θ.

Using the singular value decomposition, we can write

$$\hat{\mathbf{u}}_n = \sum_{k=1}^{\operatorname{rank}^{(t)}(\hat{\mathbf{u}}_n)} \sigma_k \mathbf{v}_k,$$

with mutually orthonormal t-rank one tensors $\mathbf{v}_k$. By the Cauchy-Schwarz inequality,

$$(\theta-\varepsilon)^2 \leq |\langle \mathbf{u}, \hat{\mathbf{u}}_0 \rangle_{\mathbf{H}}|^2 = |\langle \mathbf{u}, \hat{\mathbf{u}}_n \rangle_{\mathbf{H}}|^2 \leq \left(\sum_{k=1}^{\operatorname{rank}^{(t)}(\hat{\mathbf{u}}_n)} |\langle \mathbf{u}, \mathbf{v}_k \rangle_{\mathbf{H}}|^2 \right) \|\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2,$$

where the equality follows from (31). As $\operatorname{rank}^{(t)}(\hat{\mathbf{u}}_n) \leq (R^{(t)})^n$, we conclude using (32) that

$$\theta^2 \geq |\langle \mathbf{u}, \mathbf{v}_k \rangle_{\mathbf{H}}|^2 \geq \frac{(\theta-\varepsilon)^2}{(R^{(t)})^n \|\hat{\mathbf{u}}_n\|_{\mathbf{H}}^2} \geq \frac{(\theta-\varepsilon)^2}{(R^{(t)})^n(\theta^2 + q^{2n}(1-(\theta-\varepsilon)^2))}$$

holds for at least one k. Note that the first inequality again is due to the definition of θ. As ε can be chosen arbitrary, we obtain

$$(R^{(t)})^n(\theta^2 + q^{2n}(1-\theta^2)) \geq 1,$$

or, equivalently,

$$\theta^2(1-q^{2n}) \geq (R^{(t)})^{-n} - q^{2n} = (R^{(t)})^{-n}(1-(q^2R^{(t)})^n). \tag{33}$$

For $n \geq \frac{-\ln 2}{\ln(q^2R^{(t)})}$, which is positive by assumption, we have $(q^2R^{(t)})^n \leq 1/2$. Then (33) implies

$$\theta^2 \geq \frac{1}{(R^{(t)})^n}\frac{1-(q^2R^{(t)})^n}{1-q^{2n}} \geq \frac{1}{2(R^{(t)})^n}. \tag{34}$$

The assertion follows by simply choosing $n = \left\lceil \frac{-\ln 2}{\ln(q^2R^{(t)})} \right\rceil$. □

Note that better bounds on θ may be obtained from (34) by estimating the maximum value of the middle term as a function of n more carefully, but this quickly becomes clumsy.

The proof of Theorem 4 was based on the intuition that the ratio between the energy contraction rate q^{2n} and the reciprocal rank increase $1/(R^{(t)})^n$ after n steps of the Richardson iteration can be made arbitrarily small when $q^2R^{(t)} < 1$. Interestingly, this assumption alone does not result in better singular value decays in any of the above theorems, as only the ratio of the logarithms enters. The consideration of several steps of the fixed-point iteration only pays off when improved estimates of $R^{(t)}$ are available, as discussed for linear systems in Remark 1. An example of relevance to eigenvalue problems is given, for instance, by an operator of the form

$$\mathbf{A} = A_1 \otimes I + I \otimes A_2 + B \otimes C,$$

see also Example 1. A direct calculation reveals that for such an operator two steps of steepest descent (23) do not increase the rank by a factor of $3^2 = 9$, but only by at most 6.

5 Conclusions

We have established bounds on the singular value decays for solutions to tensor structured linear systems and eigenvalue problems. As these decays govern the low-rank approximability in various low-rank tensor formats, such as the tensor train and the hierarchical Tucker formats, our results allow to make a priori statements about the suitability of these formats to address a given application, possibly even for large orders d.

With the assumptions made in this paper, our construction yields algebraic decays. To obtain exponential decays, as they are sometimes observed in practice, further assumptions may be needed. In Remark 1, a rather restrictive commutativity assumption is shown to yield exponential decays. It would certainly be of interest to identify less restrictive assumptions.

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