

A NOTE ON NUMERICAL SINGULAR VALUES OF COMPOSITIONS WITH NON-COMPACT OPERATORS*

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Abstract. Linear non-compact operators are difficult to study because they do not exist in the finite-dimensional world. Recently, Hofmann and Mathé [Electron. Trans. Numer. Anal., 57 (2022), pp. 1–16] studied the singular values of the compact composition of the non-compact Hausdorff moment operator and the compact integral operator and found credible arguments, but no strict proof, that those singular values fall only slightly faster than those of the integral operator alone. However, the fact that numerically the singular values of the combined operator fall exponentially fast was not mentioned. In this note, we supply the missing numerical results and provide an explanation why the two seemingly contradictory results may both be true.

Key words. singular values, ill-posedness, compact operator, non-compact operator

AMS subject classifications. 15A18, 65F35

1. Introduction. For numerical computations, one often needs to find a finite-dimensional approximation to a real-world problem that can be modeled as an infinite-dimensional operator equation. A curious case is when a non-compact operator is involved in the modeling. The reason for this is that any linear operator with finite-dimensional range (in particular, discrete operators used for computations) is necessarily compact. On the other hand, whenever a non-compact operator is paired with a compact operator, the composition is compact again. It is natural to ask whether the non-compact part can “destroy” important properties of the compact one. We will investigate this in terms of the singular values.

The background of this note is the approximate solution of inverse problems. Let X and in particular Y be infinite-dimensional Hilbert spaces, and $A : X \rightarrow Y$ a bounded linear operator. An inverse problem, in the most basic definition, is to recover the cause $x^\dagger \in X$ from data $y = Ax^\dagger$, where often only a noisy approximation y^δ to y is available. Such problems become challenging when the operator A is ill-posed, as then A may not be invertible, and the (pseudo)inverse A^{-1} is discontinuous, meaning that arbitrarily small measurement errors can lead to arbitrarily large errors in the reconstruction of x^\dagger . A linear operator has a discontinuous (pseudo)inverse if and only if its range is not closed, $\mathcal{R}(A) \neq \overline{\mathcal{R}(A)}$ [2]. Nashed’s definition of ill-posedness [12] further distinguishes between ill-posedness of type I, where $\mathcal{R}(A)$ contains an infinite-dimensional closed subspace, and ill-posedness of type II, where this is not the case. In the setting where X and Y are Hilbert spaces, ill-posedness of type II occurs if and only if A is compact, and the theory for the inversion of compact linear operators has been treated abundantly in the literature; see, e.g., [2]. The degree of ill-posedness, which is of high importance for the design of appropriate regularization schemes to find reasonably good approximations to x^\dagger , is characterized by the decay of the singular values $\sigma_i(A)$ of A . Denoting by $A^* : Y \rightarrow X$ the adjoint of A , σ_i is a singular value of A if σ_i^2 is an eigenvalue of A^*A . For compact operators, the non-increasing singular values are bounded from above with $\sigma_1(A) = \|A\|$, are countable and can only accumulate in zero. The singular values and, more generally, the singular system $\{\sigma_i, u_i, v_i\}_{i=1}^\infty$, where u_i is an orthonormal basis (ONB) for $\mathcal{R}(A)$ and v_i is an ONB for $\mathcal{R}(A^*)$, is closely related to the singular value decomposition $\hat{A} = USV^T$ of a matrix approximation \hat{A} to A .

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In the Hilbert-space setting, it follows that ill-posedness of type I corresponds to non-compact operators with non-closed range. It appears that generally inverse problems with such an operator are considered less ill-posed than those with compact operators in the literature [12], but, since the operators do not possess a singular system, it is difficult to formulate an analog to the degree of ill-posedness. However, if

$$A = B \circ J$$

is a composition between a non-compact operator B and a compact operator J (note that the order in the composition does not change the statement), then A is also compact. This leads us to the main question motivating this note: Is the degree of ill-posedness of A equal to or at least similar to that of J , or can the application of the non-compact B yield a (significantly) more ill-posed problem?

We will consider only concrete choices of the operators. Our main interest for the non-compact operator is the Hausdorff-moment (HM) operator [7]

$$(1.1) \quad B^H : L^2[0, 1] \rightarrow \ell^2, \quad [B^H x]_i = \int_0^1 t^{i-1} x(t) dt.$$

Since the compact part is of less interest, we choose for simplicity the integral operator

$$(1.2) \quad J : L^2[0, 1] \rightarrow L^2[0, 1], \quad [Jx](s) = \int_0^s x(t) dt.$$

Note that the singular system of J is well known [2]; in particular, the singular values fall as $\sigma_i(J) \sim 1/i$. Finally, since the HM operator is sometimes difficult to handle, we will use the multiplication operator,

$$(1.3) \quad B^M : L^2[0, 1] \rightarrow L^2[0, 1], \quad [B^M x](s) = m(s)x(s),$$

with multiplier function $m(s)$ containing essential zeros in $[0, 1]$, to draw analogies.

Recently, the paper [5] provided some new insight on the HM operator in relation to inverse problems. Even more, Hofmann and Mathé discussed our main question in [8] from an analytical point of view. They showed that there are positive constants \underline{c} and \bar{c} such that

$$(1.4) \quad \exp(-\underline{c}i) \leq \sigma_i(B^H \circ J) \leq \frac{\bar{c}}{i}.$$

This leaves open whether the singular values fall just like those of the integration operator, or if the HM operator makes the composition exponentially ill-posed. Hofmann and Mathé then proceed to show that

$$(1.5) \quad \sigma_i(B^H \circ J) = \mathcal{O}(i^{-3/2}),$$

i.e., the composite operator is at least slightly more ill-posed than J alone, but exponential decay is not ruled out. They also provide a substantial argument, but no strict proof, that (1.5) is the actual degree of ill-posedness, and that the singular values of $A = B^H \circ J$ cannot fall exponentially fast. The reasoning for this is that the operator A^*A can be written as a Fredholm integral operator

$$(1.6) \quad [A^*Ax](s) = \int_0^1 k(s, t)x(t) dt$$

with kernel

$$(1.7) \quad k(s, t) = \sum_{j=1}^{\infty} \frac{(1-s^j)(1-t^j)}{j^2}, \quad 0 \leq s, t \leq 1.$$

While k is continuous, its derivative $\partial k(s, t)/\partial s$ has a pole at $s = 1$. In particular, k is not Lipschitz-continuous. It is well known that, for integral operators as in (1.6), exponentially decaying singular values are usually associated with $k \in C^\infty$, i.e., smooth, infinitely many times differentiable kernels. The fact that the smoothness of (1.7) is highly limited suggests that the singular values of A do not fall exponentially fast, but there seems to be no theorem available in the literature that covers this situation. Therefore, ultimately, exponential decay seems unlikely but cannot be ruled out.

What is missing in the work of Hofmann and Mathé is mention of the fact that, numerically, when $A = B^H \circ J$ is approximated by a (finite) matrix \hat{A} , its singular values do fall exponentially fast. This is somewhat surprising, in particular in comparison to the composition of J with the multiplication operator. In this case, it is well known [9, 10] that, in particular for the multiplier functions $m(s) = s^\kappa$, $\kappa > 0$ (which we will use throughout the paper), the multiplication operator does not change the degree of ill-posedness,

$$(1.8) \quad \sigma_i(B^M \circ J) \sim 1/i,$$

and numerical observations agree with this. We mention here that the operators B^H and B^M have similar properties. Both are non-compact with non-closed range, and both have a purely continuous spectrum: the interval $[0, \sqrt{\pi}]$ for B^H and all values $m(s)$, $0 \leq s \leq 1$, for B^M . With our choice of $m(s)$, the latter corresponds to the interval $[0, 1]$.

In the remainder of this paper, we make an attempt to explain this seeming mismatch. We show numerical experiments for both operators, $A = B^H \circ J$ and $A = B^M \circ J$, in Section 2. After that, we present a reasoning that allows all statements on the singular values made so far to be true without a contradiction.

2. Numerical singular values. Since the theoretical approach to the estimation of the singular values of the composite operator $A = B^H \circ J$ in [8] was not entirely conclusive, we study in this section the computed singular values of the linear systems obtained by discretizing the infinite-dimensional problems. We are mainly interested in the singular values of the composition $A = B^H \circ J$ with the Hausdorff operator B^H , but we also report on the singular values of the composition $\hat{A} = B^M \circ J$ with a multiplication operator.

To discretize the operators, we need to approximate integrals of type

$$(2.1) \quad [I_k x](s) = \int_0^1 k(s, t)x(t) dt.$$

Namely, we have (with slight abuse of notation for B^H)

$$\begin{aligned} [Jx](s) &= [I_k x](s) & \text{with } k(s, t) &= \begin{cases} 1 & t \leq s, \\ 0, & \text{otherwise,} \end{cases} \\ [B^H x]_j &= [I_k x]_j & \text{with } k(j, t) &= t^{j-1}. \end{aligned}$$

It was shown in [8] that the composition $B^H \circ J$ can be written as

$$[Ax]_j = [B^H \circ J(x)]_j = \int_0^1 \frac{1}{j} (1-t^j)x(t) dt,$$

hence

$$[Ax]_j = [B^H \circ J(x)]_j = [I_k x]_j \quad \text{with } k(j, t) = \frac{1}{j}(1 - t^{j-1}).$$

We discretize the integrals I_k with the trapezoidal rule, i.e., we use a grid $t_i, i = 1, \dots, N$, where N is given in the examples, such that $t_i = (i - 1)/(N - 1)$. Analogously, we discretize the variable $s \in [0, 1]$ as $s_j, j = 1, \dots, M$, such that

$$(2.2) \quad [I_k x](s_j) \approx \frac{1}{N-1} \left(\frac{1}{2} k(s_j, t_1) x(t_1) + \sum_{i=2}^{N-1} k(s_j, t_i) x(t_i) + \frac{1}{2} k(s_j, t_N) x(t_N) \right).$$

There are integration rules that yield a better rate of approximation of the true integral. However, we consider the trapezoidal rule as a standard implementation, and because we will see that it is enough to verify (1.8). For the Hausdorff operator, we will use a discretization fine enough to make it unlikely that the choice of integration rule alone explains the discrepancies in the singular values. We will refer back to this statement in the next section.

The discretization (2.2) yields $M \times N$ matrix approximations to the respective operators, which we indicate with a hat symbol, i.e., we have $\hat{B}^H \in \mathbb{R}^{M \times N}$ as an approximation to (1.1), $\hat{J} \in \mathbb{R}^{M \times N}$ as an approximation to (1.2), and $\hat{A} \in \mathbb{R}^{M \times N}$ as an approximation to the composition $A = B^H \circ J$. Finally we have the multiplication operator B^M from (1.3), which is approximated through a diagonal matrix \hat{B}^M with entries $\hat{B}^M(i, i) = m(t_i), i = 1, \dots, N$. Note that, due to discretization, the representations \hat{B}^M and \hat{B}^H are compact, whereas the infinite-dimensional operators are not. We can therefore calculate the singular values for the discretized operators.

Our first study is on the singular values of the composite operator \hat{A} as a discrete approximation to the (compact) composition $A = B^H \circ J$. We choose $N = M = 10\,000$ and use MATLAB to compute the first 20 singular values of the matrices, as this is sufficient to convey the message. Figure 2.1 shows that the singular values of \hat{A} decay exponentially fast, as in the half-logarithmic scale exponential decay appears linear. It is curious to note that $\sigma_i(\hat{A}) \propto \sigma_i(\hat{B}^H) \sigma_i(\hat{J})$, since, for general operators $A : X \rightarrow Z, B : Z \rightarrow Y$, one can only guarantee that

$$(2.3) \quad \sigma_{2i}(AB) \leq \sigma_i(A) \sigma_i(B);$$

see [13]. It is also important to mention that in Figure 2.1 we clearly have $\sigma_i(\hat{J}) \sim 1/i$, so, for the compact operator J , theory and numerics agree. We conclude from this that, numerically, the Hausdorff moment problem, even in composition with the integration operator, is exponentially ill-posed. We remark that this is true, in fact even more pronounced, when we use fewer than 10 000 discretization points or moments. We will come back to this in Section 3 below.

As a comparison, we now replace the Hausdorff moment operator with the multiplication operator, which is known to preserve the ill-posedness of the integration operator. Figure 2.2 shows that the singular values of the discretized composite operator $\hat{A} = B^M \circ J$ do not fall exponentially fast, but stay close to the rate i^{-1} known from the theory. In this example we can calculate more singular values, and doing so we clearly see that $\sigma_i(\hat{A}) \sim \sigma_i(\hat{J}) = 1/i$. This result has been reported before in [3], but the contrast to the HM operator is still surprising. Before we make an attempt at an explanation for this discrepancy in the next section, we proceed with another numerical experiment.

The second indicator for the estimation of the decay of the singular values in [8] was the smoothness of the kernel $k(s, t)$ from (1.7) and the singular values of the associated integral

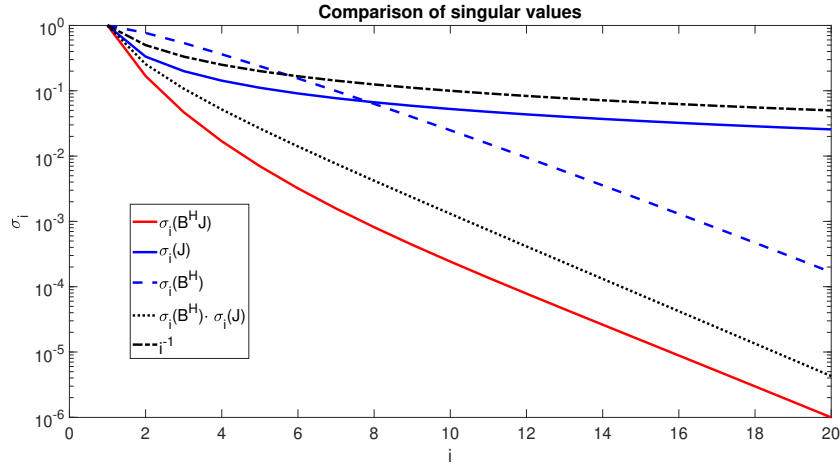


FIG. 2.1. Singular values σ_i of the discrete operators \hat{J} , \hat{B}^H , and \hat{A} , and the reference line for polynomial decay i^{-1} .

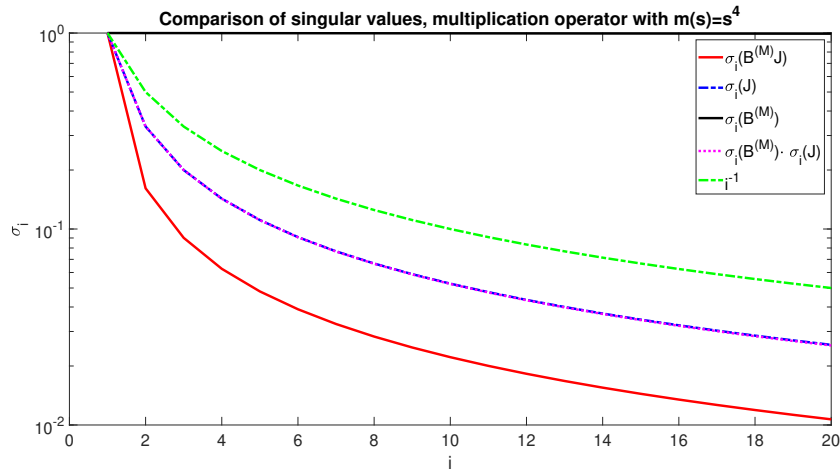


FIG. 2.2. Singular values σ_i of the discrete operators \hat{J} , \hat{B}^M with $m(s) = s^4$, and \hat{A} as discretization of $A = B^M \circ J$, and reference line for polynomial decay $\sigma_i = i^{-1}$.

operator $[A^*Ax](s) = \int_0^1 k(s,t)x(t) dt$. We discretize this as a special case of the integral $I_k[x](s)$ from (2.1) with $M = N = 5000$ supporting points for s and t , respectively. As cut-off for the summation in the kernel, we chose several values of j_{\max} up to $j_{\max} = 200\,000$. The results are given in Figure 2.3. We see that the singular values σ_i increase slowly with increasing j , but even with j_{\max} they fall exponentially fast. For comparison, we also plotted the singular values $\sigma_i(\hat{A})^2$, where $\sigma_i(\hat{A})$ are directly taken from Figure 2.1. From theory it is known that $\sigma_i(A)^2 = \sigma_i(A^*A)$, and we indeed obtain a reasonable fit. We also plotted the theoretical value $\sigma_i(A^*A) \sim i^{-3}$ from [8], which is clearly not met.

As we have seen, all numerical experiments, even with a fairly large number of discretization points, indicate an exponential decay of the singular values of the discretized composite operator $A = B^H \circ J$. Whether this is due to the singular values decaying exponentially

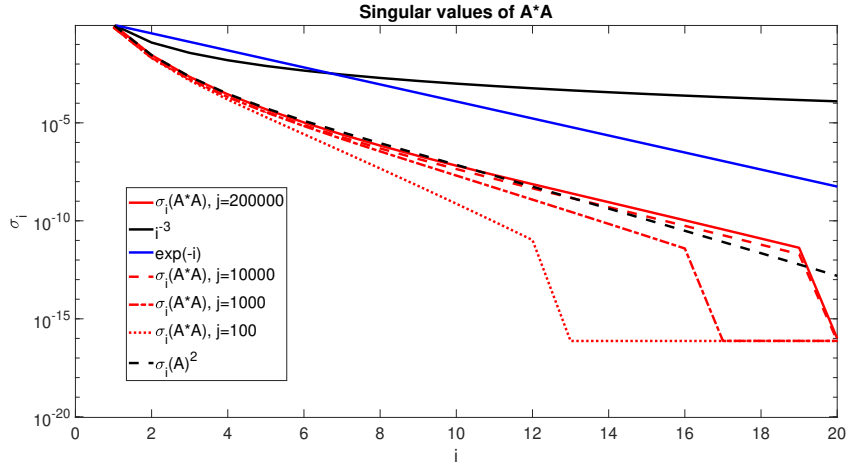


FIG. 2.3. Singular values of A^*A from (1.6) with truncation indices $j_{\max} \in \{100, 1000, 10\,000, 200\,000\}$. The singular values increase with j_{\max} , although the difference between $j_{\max} = 10\,000$ and $j_{\max} = 200\,000$ is almost negligible. The decay rate $\sigma_i \sim i^{-3}$ implied by the upper bound in (1.4) could not be observed, as we always saw a much faster decay of the singular values. However, we have a good fit to the squared singular values $\sigma_i^2(A)$ previously computed and shown in Figure 2.1. Note that, numerically, $\text{rank}(A^*A)$ is between 13 and 20 here.

fast also in the infinite setting, or due to numerical effects, can still not be answered with certainty. Below, we present an argument that suggests the latter and might reconcile theory and numerics.

3. Explaining the seeming inconsistency. The focus in this section is on the singular values of the discrete approximations to the non-compact operators B^H and B^M .

For the Hausdorff operator B^H , we recall from [5] that B^H can be seen as a Cholesky factor of the Hilbert matrix, as it was shown that $B^H = LQ$, where $Q : L^2[0, 1] \rightarrow \ell^2$ is an isometry and L is triangular with $LL^T = H$ where H is the Hilbert matrix,

$$H_{ij} = \left(\frac{1}{i+j-1} \right)_{i,j=1}^{\infty}.$$

For an explicit formula for the entries L_{ij} , we refer to [5]. The Hilbert matrix H , as an infinite-dimensional matrix mapping from ℓ^2 to ℓ^2 , is non-compact with purely continuous spectrum $[0, \pi]$ [11]. In the discrete setting, we truncate H and L to the first n rows and denote these objects by H_n and L_n . One has $\sigma_i(H_n) = \sigma_i(L_n)^2$. Note that no integrals are needed for the entries of the operators L, L_n and H, H_n . Since the isometry Q in the decomposition $B^H = LQ$ does not change the singular values, we conclude that the integration method used to approximate $A = B^H \circ J$ in the previous section is not crucial for the determination of the singular values and that the behavior of the numerical singular values is more deeply rooted in the operator B^H and the closely related matrices L_n .

A big advantage of the identities above is that we can use results on the rather well-studied Hilbert matrix and its truncation, for which we have good knowledge of the smallest and largest singular values, but lack details in between. More precisely, we have $\|H\|_{\ell^2 \rightarrow \ell^2} = \pi$ [14], and H_n has, for sufficiently large n , eigenvalues arbitrarily close to π . This follows by setting $x_r = 1/\sqrt{r}$ for $r = 1, \dots, N$, and $x_r = 0$ for $r > N$, and observing that $\langle Hx_r, x_r \rangle_{\ell^2 \times \ell^2} / \|x_r\|^2 \rightarrow \pi$ as $N \rightarrow \infty$ [6, Theorem 323 and following pages]. As a consequence, it follows that $\|H_n\| \rightarrow \pi$ as $n \rightarrow \infty$, and $\sigma_1(H_n) \rightarrow \pi$. It is also well known

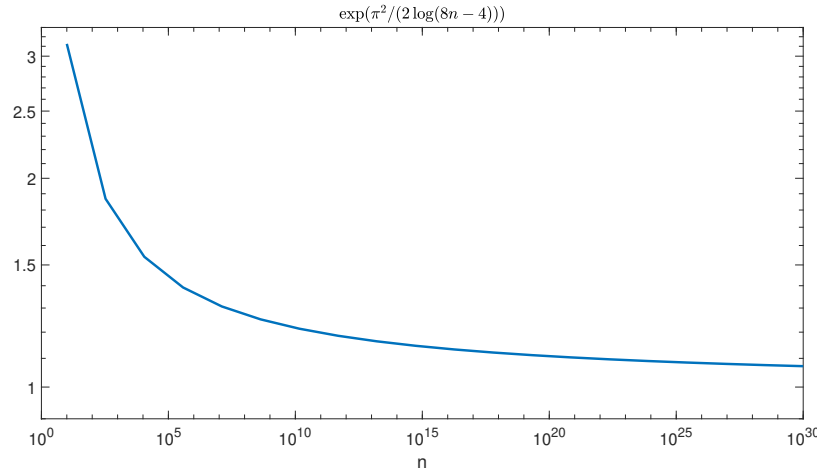


FIG. 3.1. Plot of the exp term in (3.1) as a function of n . The convergence is extremely slow.

that the smallest eigenvalue of the truncated Hilbert matrix H_n is $\sigma_n(H_n) \sim \exp(-3.526n)$; see, e.g., [14]. However, a precise characterization of the intermediate singular values seems to be missing. A valuable hint, however, can be found in [1]. There it was shown that

$$(3.1) \quad \sigma_{i+1}(H_n) \leq 4 \left[\exp\left(\frac{\pi^2}{2 \log(8n - 4)}\right) \right]^{-2i} \sigma_1(H_n), \quad 1 \leq i \leq n - 1.$$

Since we could not find a lower bound on $\sigma_{i+1}(H_n)$, the following arguments involve some speculation, but another comparison to the multiplication operator at the end of the section makes them appear reasonable. First, note that $\sigma_1(H_n) \leq \pi$ for all n , so this factor is not of interest. Next, we remark that, for fixed n , (3.1) yields exponential decay of the singular values of H_n . Because of (2.3), we have

$$(3.2) \quad \sigma_{2i}(\hat{B}^H \hat{J}) \leq \sigma_i(L_n) \sigma_i(\hat{J}) \leq 2 \left[\exp\left(\frac{\pi^2}{2 \log(8n - 4)}\right) \right]^{-i} \sqrt{\pi} \frac{1}{i},$$

which shows that the singular values of the discrete approximation to $B^H \circ J$ fall exponentially and further supports our claim that the results of our numerical experiment in Section 2 is correct and not due to incorrect approximation of the integrals.

The upper bound in (3.1) depends on the truncation index n . The term in brackets decreases monotonically with

$$\lim_{n \rightarrow \infty} \exp\left(\frac{\pi^2}{2 \log(8n - 4)}\right) = 1.$$

However, the convergence is extremely slow; see the plot in Figure 3.1. For $n = 10^{30}$ the term has the value 1.072.

In the limit $n \rightarrow \infty$, (3.1) therefore reduces to $\sigma_{i+1}(H_n) \leq 4\sigma_1(H_n)$, and because $\sigma_i(H_n) \leq \sigma_1(H_n) \leq \|H_n\| \leq \pi$, we even have $\sigma_i(H_n) \leq \pi$. We conjecture that indeed every singular value (with fixed index) converges slowly to π ,

$$(3.3) \quad \lim_{n \rightarrow \infty} \sigma_i(H_n) = \pi.$$

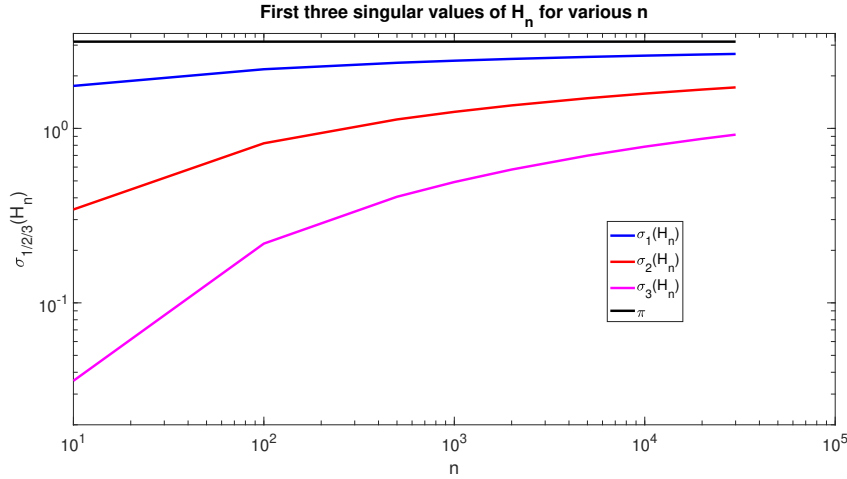


FIG. 3.2. Singular values of the truncated Hilbert matrix for various values of n . As n increases, each singular value increases.

Numerically, we see that, for each index i , the singular values $\sigma_i(H_n)$ as functions of n are increasing; see Figure 3.2. However, likely due to the convergence of the \exp term of (3.1) as plotted in Figure 3.1, we cannot increase the discretization enough to approach the limit, since no computer can hold such a matrix. Nevertheless, the increase of the singular values we can observe adds plausibility to (3.3).

Below, we will prove a result analogous to (3.3) for the multiplication operator. Before that, we discuss further consequences of (3.1). In the limit $n \rightarrow \infty$ we obtain from (3.2) the upper bound $\sigma_{2i}(\hat{B}^H \hat{J}) \leq 2\sqrt{\pi}/i$. This is the same upper bound as on the right-hand side of (1.4) in the infinite-dimensional setting. However, in the infinite-dimensional setting, we also know the sharper bound $i^{-3/2}$ from (1.5). Whether this means that the bound in (3.1) is not sharp or if the discrepancy is perhaps due to the index shift (note the index $2i$ on the left-hand side of (1.5)) is not clear at this point. However, we conclude that the exponential decay of the singular values observed in the numerical experiments does not invalidate the claim of polynomial decay made in [8], despite the huge gap. In fact, one can see numerically that, similarly to those of the truncated Hilbert matrix in Figure 3.2, the singular values of \hat{A} increase (again very slowly) when the discretization is refined; see Figure 3.3.

We close this section by checking analogies of the above results for the multiplication operator. As mentioned before, the spectrum of B^M consists of all values of the multiplier function $m(s)$, $0 \leq s \leq 1$. Due to the simple structure of the multiplication operator, we can prove that each singular value of its discrete approximation converges to a specific value, so the analog of the conjecture (3.3) is true for B^M .

LEMMA 3.1. *Let $m(s) \in L^\infty[0, 1]$ be the multiplier function of the operator B^M from (1.3) with $m_{\max} := \text{ess sup}_{s \in [0, 1]} m(s) < \infty$. Let $s_k = (k-1)/(K-1)$, $k = 1, \dots, K$, $K \in \mathbb{N}$, be discretizations of the interval $[0, 1]$ in K points. Then the diagonal matrices \hat{B}^M with entries $\hat{B}^M(k, k) = \tilde{m}(s_k)$, where $\tilde{m}(s_k)$ is the decreasing rearrangement of $m(s_k)$, and zero outside the diagonal, are a discrete approximation to B^M and*

$$\lim_{K \rightarrow \infty} \sigma_i(\hat{B}^M) = m_{\max}.$$

for each $i \in \mathbb{N}$.

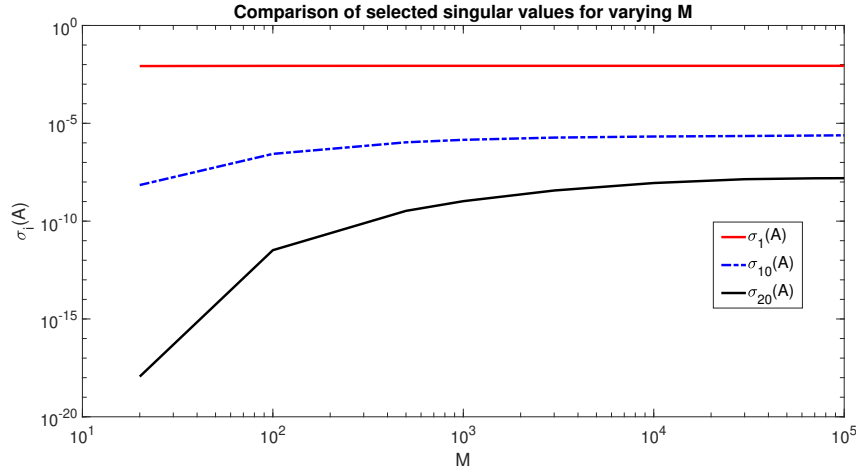


FIG. 3.3. Singular values $\sigma_1(\hat{A})$, $\sigma_{10}(\hat{A})$, and $\sigma_{20}(\hat{A})$ as a function of the maximal moment discretization M . It appears that the singular values converge with increasing M .

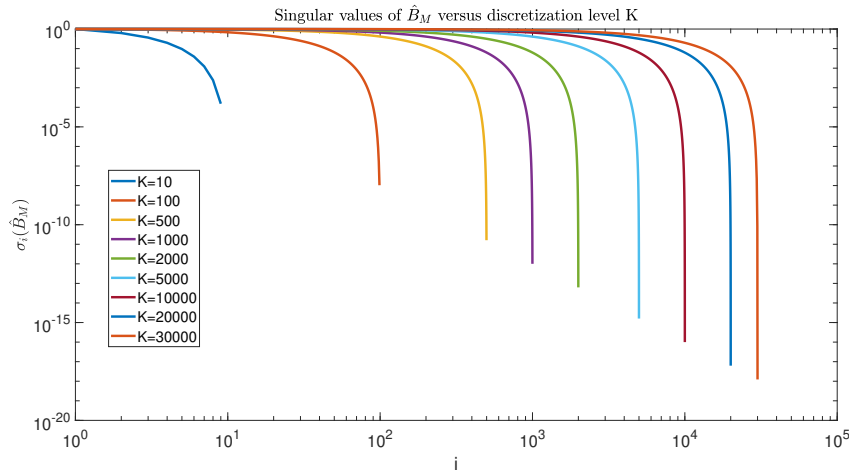


FIG. 3.4. Singular values of the discrete multiplication operator \hat{B}^M with $m(s) = s^4$ for various values of N . As N increases, each singular value converges to 1.

Proof. Because \hat{B}^M is diagonal, its singular values are the decreasing rearrangement of the diagonal entries. Without loss of generality, we consider $m(s)$ to be decreasing further. Because $s_k - s_{k-1} \rightarrow 0$ as K increases, there is a $\bar{K} = \bar{K}(i, \epsilon)$ such that, for each fixed i and arbitrary but fixed $\epsilon > 0$, one has $\sigma_i(\hat{B}^M) = m(s_i) > m_{\max} - \epsilon$ for $K > \bar{K}$. \square

Numerically, this can be confirmed easily. Since the singular values of the discretized multiplication operator are trivial, we can plot them all. We have done so in Figure 3.4 for varying K . For each fixed index i , we see that $\sigma_i(\hat{B}^M) \rightarrow 1$ as the discretization level K increases. The relation (2.3) hence yields the bound $\sigma_{2i}(\hat{B}^M \circ \hat{J}) \leq \sigma_i(\hat{B}^M)\sigma_i(\hat{J}) \sim 1/i$ when B^M is discretized fine enough.

To summarize this section and conclude the paper, we have demonstrated the possibility that the numerically observed exponentially decaying singular values of the composition

$A = B^H \circ J$ can be explained through the very slow numerical convergence of the spectrum of the discrete approximations in terms of discretization level. Our results suggest that using a discretization level that is impossible to realize, one might see singular values dropping only (approximately) polynomially fast. In this sense, the results of [8] do not contradict our experiments in Section 2. Yet, despite all efforts, several open questions surrounding the Hausdorff moment problem and its composition with a compact operator remain unanswered. We have gathered and stated them prominently in [4].

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