Any Circulant-Like Preconditioner for Multilevel Matrices Is Not Optimal

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ABSTRACT

Optimal preconditioners (those that provide a proper cluster at 1) are very important for the cg-like methods since they make them converge superlinearly. As is well known, for Toeplitz matrices generated by a continuous symbol, many circulant and circulant-like (related to different matrix algebras) preconditioners were proved to be optimal. In contrast, for multilevel Toeplitz matrices, there has been no proof of the optimality of any multilevel circulants. In this paper we show that such a proof is not possible since any multilevel circulant preconditioner is not optimal, in the general case of multilevel Toeplitz matrices. Moreover, for matrices not necessarily Toeplitz, we present some general results that enable us to prove that many popular structured preconditioners can not be optimal.

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1 Introduction

The phenomenon of superlinear convergence for the cg-like methods was scrutinized, first of all, in [1, 22], and then it has become one of most topical subjects in many papers discussing how to make the cg-like iterations converge superlinearly [6, 8, 12, 13, 14, 15, 16, 17, 23, 24]. The key concept behind these papers is that of a cluster. From some naive approach in the beginning, it has eventually developed into a rigorous notion [4, 25, 26, 28, 29] as follows.

Consider a sequence of matrices $A_n \in \mathbb{C}^{n\times n}$ and a set M in the complex plane. Denote by M_ε the ε-extension of M, which is the union of all balls of radius ε centered at points of M. Let $\gamma_n(\varepsilon)$ count those eigenvalues of A_n that do not belong to M_ε. Assume that, for any $\varepsilon > 0$,

$$\gamma_n(\varepsilon) = o(n), \quad n \to \infty.$$

Then M is called a general (some say weak) cluster. If $o(n) = O(1)$, then M is called a proper (some say strong) cluster.

Of course, we are interested in the clusters as narrow as possible. In this paper we deal only with one-point clusters, and mostly those of the singular values rather than eigenvalues.

If A_n are Hermitian positive definite matrices and C_n are their Hermitian positive definite precondintioners, then the superlinear convergence for the preconditioned conjudate gradient (pcg) method is guaranteed whenever the eigenvalues of $C_n^{-1}A_n$ have a proper cluster at 1. In the non-Hermitian case, the pcg-method can be applied to the symmetrized preconditioned system, and the superlinear convergence is seen so long as the singular values of $C_n^{-1}A_n$ have a proper cluster at 1.

We would have called a preconditioner C_n for A_n optimal if the singular values of $C_n^{-1}A_n$ have a proper cluster at 1. However, we will require a little more.

A preconditioner C_n for A_n is said to be *suboptimal* if the singular values of $C_n^{-1}A_n - I_n$ have a cluster at 0 (I_n is the identity matrix of order n), and *optimal* if this cluster at 0 is proper.

There are also useful equivalent definitions in the terms of convenient matrix relations. A preconditioner C_n for A_n is suboptimal iff, for any $\varepsilon > 0$, there exist matrices $E_{n\,\varepsilon}$ and $R_{n\,\varepsilon}$ such that

$$C_n^{-1} A_n - I_n = E_{n\,\varepsilon} + R_{n\,\varepsilon} \tag{1}$$

with

$$||E_{n\,\varepsilon}||_2 \le c_1(\varepsilon), \qquad \lim_{\varepsilon \to 0} c_1(\varepsilon) = 0; \tag{2}$$

$$\operatorname{rank} R_{n\,\varepsilon} \le c_2(n, \varepsilon), \qquad \lim_{n \to \infty} \frac{c_2(n, \varepsilon)}{n} = 0 \quad \forall\, \varepsilon > 0. \tag{3}$$

A suboptimal preconditioner C_n is optimal iff $c_2(n, \varepsilon)$ is uniformly bounded in n (which is equivalent to the claim that some bound c_2 does not depend on n, and so we may write $c_2 = c_2(\varepsilon)$).

For the singular values of $C_n^{-1} A_n$, it is easy to prove that a suboptimal preconditioner provides a general cluster at 1 while an optimal one provides a proper cluster, and thence the superlinear convergence. However, beware of claiming the reverse, because a preconditioner providing a proper cluster at 1 for the singular values of $C_n^{-1} A_n$ is not necessarily optimal according to our definition.

In applications, optimal preconditioners may be not easily available. Still, there are some important cases when they are.

If $A_n = A_n(f) = [a_{i-j}]_{ij=1}^n$ are Toeplitz matrices associated with an absolutely convergent Fourier series for a positive symbol

$$f(x) = \sum_{k=-\infty}^{\infty} a_k e^{\mathrm{i}kx},$$

then the circulant preconditioners proposed by G. Strang and T. Chan are optimal [4]. More precisely, this is true for the G. Strang preconditioner when f belongs to the Dini-Lipschitz class [18], while for the T. Chan this is true when f is merely continuous [5, 18, 19]. Moreover, many other preconditioners related to different matrix algebras [2, 3, 9, 11, 19, 20, 21] can be proved to be optimal even in the ill-conditioned case where the symbol f has zeros [7, 18].

From the practical point of view, the profusion of research devoted to preconditioners for Toeplitz matrices is likely to go with the hope to use the same ideas for multilevel Toeplitz matrices (see [24]). In the multilevel case, the constructions similar to those of the unilevel case have led only to sub-optimal preconditioners [26, 19].

As yet, all attempts to construct an optimal multilevel circulant or circulant-like preconditioner ended with nothing. In this paper, we show that this is not because we have not seized the idea how to prove this. It can not be proved because it is not true in the general case.

We propose thus a negative result that can be summarized as follows. If a preconditioner C_n for A_n is sought in the form $C_n = U_n D_n V_n$, with unitary matrices U_n and V_n (still subject to some assumptions) given beforehand and so independent of A_n, and a diagonal matrix D_n to be chosen, then there are multilevel Toeplitz matrices A_n associated with a multivariate symbol, for which the preconditioner C_n can not be optimal.

All the same, much of what we discuss has little to do with the Toeplitz property itself; we use, instead, some general ergodic assumptions (that follow from the Szego-like theorems in the Toeplitz case). Moreover, our results might apply also to the preconditioners for unilevel matrices.

In Section 2, we present the basic theoretical tools allowing us to prove that a preconditioner is not optimal. Then, in Section 3, we recollect the notion, common toolkit, and some ergodic results for the multilevel matrices. In Section 4, we present our main negative results concerning optimal circulant-like preconditioners.

2 Basic statements

All matrices, for the time being, are unilevel of order n (with different n). The next two lemmas are almost evident, so they go without a proof.

Lemma 2.1 *Assume that matrices C_n are nonsingular and uniformly bounded in n, in the spectral norm, together with C_n^{-1}. Then a preconditioner C_n for A_n is suboptimal iff the singular values of $A_n - C_n$ have a general cluster at zero, and it is optimal iff this cluster is proper.*

We will say that A_n and C_n are ε-close up to the rank bound $r = r(n, \varepsilon)$ if, $\forall\, \varepsilon > 0$ and $\forall\, n$, there exist matrices $E_{n\,\varepsilon}$ and $R_{n\,\varepsilon}$ such that

$$A_n - C_n = E_{n\,\varepsilon} + R_{n\,\varepsilon}, \quad ||E_{n\,\varepsilon}||_2 \le \varepsilon, \quad \operatorname{rank} R_{n\,\varepsilon} \le r(n, \varepsilon). \tag{4}$$

Lemma 2.2 *The singular values of $A_n - C_n$ have a cluster at zero iff the matrices A_n and C_n are ε-close up to the rank bound $r(n, \varepsilon)$ which enjoys the relation*

$$\lim_{n \to \infty} \frac{r(n, \varepsilon)}{n} = 0 \quad \forall\, \varepsilon > 0. \tag{5}$$

The cluster at zero is proper iff $r(n, \varepsilon)$ does not depend on n.

We term a matrix *equimodular* if all its entries are equal in modulus. It is clear that any unitary equimodular matrix of order n has all its entries equal to $1/\sqrt{n}$ in modulus.

Lemma 2.3 *Let $C_n = U_n D_n V_n$, where matrices D_n are diagonal, U_n and V_n are unitary, and V_n are equimodular. Assume that, for any $\varepsilon > 0$ and for any n, there exists a column $e_{\varepsilon\, n}$ of I_n such that $||C_n e_{\varepsilon\, n}||_2 \le \varepsilon$. Then the singular values of C_n are clustered at zero.*

Proof. If $D_n = \operatorname{diag}\{d_{1n}, \ldots, d_{nn}\}$, then the singular values of C_n are equal to $|d_{jn}|$, $1 \le j \le n$. From the contrary, assume that zero is not a cluster for them. Then, there are positive δ and c such that

$$\gamma_n(\delta) \ge cn \tag{6}$$

for infinitely many n. In line with the previous notation, $\gamma_n(\delta)$ counts those indices j for which $|d_{jn}| > \delta$. Take up any n for which (6) is valid, and set $v_n = [v_{1n}, \ldots, v_{nn}]^T \equiv V_n\, e_{\varepsilon\, n}$. Then, for those n,

$$||C_n e_{\varepsilon\, n}||_2 \;=\; ||D_n v_n||_2 \;=\; \sqrt{\sum_{j=1}^{n} |d_{jn} v_{jn}|^2} \;\ge\; \sqrt{c}\, \delta,$$

and hence, this can not be less than ε for an arbitary $\varepsilon > 0$. $\square$

We will say that A_n are ε-zeroed on $\rho = \rho(n, \varepsilon)$ columns of the identity matrix I_n if, first, they are uniformly in n bounded in the spectral norm, and second, $\forall\, \varepsilon > 0$ and $\forall\, n$, for some $\rho(n, \varepsilon)$ columns $e_{jn\,\varepsilon}$ of I_n it holds that

$$||A_n\, e_{jn\,\varepsilon}||_2 \ \leq \ \varepsilon, \quad j = 1, \, \ldots \, , \rho(n, \varepsilon).$$

Lemma 2.4 *Let matrices A_n and C_n be ε-close with the rank bound $r(n, \varepsilon)$, and let A_n be ε-zeroed on $\rho(n, \varepsilon)$ columns of I_n so that*

$$\lim_{n \to \infty} \frac{r(n, \varepsilon)}{\rho(n, \varepsilon)} = 0. \tag{7}$$

Suppose $||C_n||_2$ are uniformly bounded in n. Then, $\forall\, \varepsilon > 0$ and $\forall\, n$, there is a column $e_{n\,\varepsilon}$ of I_n such that

$$||C_n\, e_{n\,\varepsilon}||_2 \ \leq \ 3\,\varepsilon.$$

Proof. By contradiction, assume that

$$||C_n\, e_{jn\,\varepsilon}||_2 \ > \ 3\,\varepsilon, \quad j = 1, \, \ldots \, , \rho(n, \varepsilon).$$

Since A_n are ε-zeroed on the vectors $e_{jn\,\varepsilon}$, it implies that

$$||(A_n - C_n)\, e_{jn\,\varepsilon}||_2 \ > \ 2\,\varepsilon.$$

Denote be $\sigma_{1n} \geq \ldots \geq \sigma_{nn}$ the singular values of $A_n - C_n$. Then, as is well known,

$$\sum_{j=1}^{\rho} \sigma_{jn}^2 \ \geq \ \sum_{j=1}^{\rho} ||(A_n - C_n)\, e_{jn\,\varepsilon}||_2.$$

Since A_n and C_n are ε-close up to the with the rank bound $r(n, \varepsilon)$, it follows that

$$\sigma_{jn} \leq \varepsilon \quad \text{for} \quad j > r = r(n, \varepsilon).$$

Using this and taking into account the preceding inequalities, we obtain

$$r\; \sigma_{1n}^2 \ \geq \ 4\varepsilon^2 \cdot \rho - \varepsilon^2\, (\rho - r),$$

and thence

$$\frac{r(n,\varepsilon)}{\rho(n,\varepsilon)}\,||A_n - C_n||_2^2 \;\geq\; 3\,\varepsilon^2.$$

On the strength of (7) and since the spectral norms of the matrices are bounded, the right-hand side must vanish as $n \to \infty$, which is at odds with the last inequality. □

Theorem 2.1 *Suppose that $C_n = U_n D_n V_n$, where matrices D_n are diagonal, U_n and V_n are unitary, and V_n are equimodular. Let matrices A_n and C_n be ε-close with the rank bound $r(n,\varepsilon)$, and let A_n be ε-zeroed on $\rho(n,\varepsilon)$ columns of I_n. If the singular values of A_n are not clustered at zero, then (7) does not stand, that is,*

$$r(n,\varepsilon) \quad \neq \quad o(\rho(n,\varepsilon), \qquad n \to \infty. \tag{8}$$

Proof. We do not lose generality if assume that C_n are bounded in the spectral norm uniformly in n. If it is not the case, we transfer to another matrices $\tilde{C}_n$ satisfying the same premises with $r(n,\varepsilon)$ being possibly replaced by $2\,r(n,\varepsilon)$. Indeed, the number of singular values for C_n that are greater than $||A_n||_2 + \varepsilon$ can not exceed $r(n,\varepsilon)$, and we may thus get to $\tilde{C}_n$ by cutting off the largest diagonal entries of D_n in the equation $C_n = U_n D_n V_n$.

Assume that the relation (7) is still fulfilled. Then, since all the premises of Lemma 2.4 are fulfilled, we conclude that, for any $\varepsilon > 0$ and for any n, there exists a column $e_{\varepsilon n}$ of I_n such that $||C_n e_{\varepsilon n}||_2 \leq \varepsilon$. From Lemma 2.3, we now deduce that the singular values of C_n have a cluster at zero.

Allowing for (7), we have also $r(n,\varepsilon) = o(n)$, which implies that A_n and C_n have the same clusters [26, 29]. However, the matrices A_n have no singular value cluster at zero, and this can not be reconciled with the above conclusion that C_n have the cluster at zero. □

Theorem 2.2 *Under the hypotheses of Theorem 2.1, assume that*

$$\lim_{n\to\infty} \rho(n,\varepsilon) = \infty \qquad \forall\, \varepsilon > 0.$$

Then the singular values of $A_n - C_n$ can not have a proper cluster at zero.

Proof. From Lemma 2.2, $r(n,\varepsilon)$ is bounded uniformly in n. Then, obviously, $r(n,\varepsilon) = o(\rho(n,\varepsilon))$, which contradicts (8). □

Theorem 2.3 *Under the hypotheses of Theorem 2.2, consider any matrices P_n such that $P_n + A_n$ and $P_n + C_n$ are nonsingular and uniformly bounded in n, in the spectral norm, together with their inverses. Then the matrices $P_n + C_n$ can not be optimal preconditioners for $P_n + A_n$.*

Proof. According to Lemma 2.1, the preconditioner $P_n + C_n$ for $P_n + A_n$ is optimal iff the singular values of $A_n - C_n$ have a proper cluster at zero. All reduces now to applying Theorem 2.2. $\Box$

It might be useful to consider also *quasi-equimodular* matrices, instead of equimodular ones. A matrix $V = [v_{ij}]$ of order n is referred to as quasi-equimodular if

$$\frac{c_1}{\sqrt{n}} \;\le\; |v_{ij}| \;\le\; \frac{c_2}{\sqrt{n}} \quad \forall\, i, j,$$

for some $0 < c_1 \le c_2$ independent of n. It is transparent that the above statements remain valid for quasi-equimodular matrices.

However, the same statements stand also even in a more general case of *subequimodular* matrices. This notion applies to a sequence of matrices, not to an individual matrix.

A sequence of matrices $V_n = [v_1^n, \ldots, v_n^n]$ is said to be subequimodular if, for any sequence of indices $j(n)$, $1 \le j(n) \le n$, $n = 1, 2, \ldots$, there exists $\delta > 0$ such that the set $[\delta, +\infty]$ is a cluster for $|v_{1\,j(n)}|, \ldots, |v_{n\,j(n)}|$, the absolute values of the entries of the column $j(n)$. It is not difficult to show that the above statements hold true for subequimodular matrices V_n.

3 Multilevel preliminaries

We call a matrix multilevel if it can be viewed as one with a nested block structure: A is a p-level matrix of multiorder $n = (n_1, \ldots, n_p)$, if it is a matrix with $n_1 \times n_1$ blocks, each of them consists of $n_2 \times n_2$ blocks, and so on. Hence, A is of order $N(n) \equiv n_1 \ldots n_p$. The rows and columns of A can be naturally pointed to through multiindices $i = (i_1, \ldots, i_p)$ and $j = (j_1, \ldots, j_p)$. Thus,

$$A = [a_{ij}], \quad 1 \le i, j \le n,$$

where $1 = (1, \ldots, 1)$, and inequalities between multiindices are understood in the entrywise sense.

Multilevel matrices may possess some structure: A_n is called a p-level Toeplitz matrix if $A_n = [a_{i-j}]$, and A_n is called a p-level circulant if $A_n = [a_{i-j\,(\mathrm{mod}\,n)}]$, where $i(\mathrm{mod}\,n) \equiv (i_1(\mathrm{mod}\,n_1),\ \ldots\ , i_p(\mathrm{mod}\,n_p))$.

Given two sequences of p-level matrices A_n and B_n of multiorder n, we call their singular values equally distributed if, for any function F continuous with a bounded support,

$$\frac{1}{N(n)}\Sigma(A_n, F) - \frac{1}{N(n)}\Sigma(B_n, F) = o(1), \quad n \to \infty,$$

where

$$\Sigma(A_n, F) \equiv \sum_{1 \le i \le n} F(\sigma_i(A_n)),$$

and $n \to \infty$ means that every component of the multiindex n tends to infinity.

The singular values of multilevel matrices A_n are called distributed as $f(z)$ for $z \in \Pi$, if, for any F continuous with a bounded support,

$$\frac{1}{N(n)}\Sigma(A_n, F) \to \frac{1}{\mathrm{mes}\,\Pi} \int_\Pi F(f(z))dz.$$

Here, Π is a Lebesgue-measurable set and f is a Lebesgue-measurable function on Π.

If $f(z) = 1$, then the above means that the singular values of A_n have a general cluster at 1. It is not necessarily a proper cluster.

Let $z \in \Pi \equiv [-\pi, \pi]^p$, and consider $f \in L_1(\Pi)$ with the formal Fourier expansion

$$f(z) \sim \sum_k a_k\, e^{\mathrm{i}(k,z)},$$

where

$$k = (k_1, \ldots, k_p), \quad (k, z) = k_1 z_1 + \ldots + k_p z_p.$$

Such a function f (we call it a symbol) generates naturally the p-level Toeplitz matrices as follows:

$$A_n(f) = [a_{i-j}], \quad 1 \le i, j \le n.$$

For the unilevel Hermitian Toeplitz case, the classical distribution results can be found in [10]. The Szego-like theorem for the singular values of $A_n(f)$

obtained in [27] reads: if a symbol $f \in L_1(\Pi)$ is a complex-valued function of $z \in \Pi = [-\pi, \pi]^p$, then the singular values of $A_n(f)$ are distributed as $|f(z)|$ with $z \in \Pi$.

4 Main negative results

Consider a p-variable symbol $f(x_1, \ldots, x_p) = \frac{1}{2}\ \exp\{\mathrm{i}x_1 + \ \ldots\ \mathrm{i}x_p\}$ and the corresponding p-level Toeplitz matrices $A_n = A_n(f)$, where $n = (n_1, \ldots, n_p)$.

Theorem 4.1 *For $I_n + A_n$, any preconditioner of the form $I_n + C_n$, where C_n is a p-level circulant, is not optimal.*

Proof. As is not difficult to verify, the matrices A_n are zeroed (ε-zeroed with $\varepsilon = 0$) on $\rho(n)$ columns of the identity matrix of order $N(n) = n_1 \ldots n_p$, where

$$\rho(n) \ \geq \ c\, N(n) \sum_{k=1}^{p} \frac{1}{n_k}, \tag{9}$$

and $c \geq 2^{1-p}$ provided that $n_k \geq 2$ for all k. Clearly, $\rho(n) \to \infty$ as $n \to \infty$ (which means, by definition, that every n_k tends to infinity). Note also that $C_n = V_n^* D_n V_n$, where V_n is a unitary equimodular matrix, for it is the Kronecker product of Fourier matrices. Therefore, we may have recourse to Theorem 2.3, and this completes the proof. $\square$

In effect, the above proof enables us to claim much more. In particular, we can propose a lower estimate on the rank of $R_{n\,\varepsilon}$ in the splitting for $A_n - C_n$ concerning the ε-closeness of A_n and C_n. What is more, it is possible to cover a more general case when C_n is not necessarily a multilevel circulant. We call matrices C_n *ciculant-like* if, for any n, it holds that $C_n = V_n^* D_n V_n$, where D_n is a diagonal matrix, and matrices V_n are unitary subequimodular matrices.

Theorem 4.2 *For $I_n + A_n$, any suboptimal preconditioner of the form $I_n + C_n$, where C_n are p-level circulant-like matrices, provides the singular value cluster for which, for some $c(\varepsilon) > 0$ and infinitely many n, it holds*

$$\gamma_n(\varepsilon) \ \geq \ c(\varepsilon)\ \rho(n),$$

where $\rho(n)$ is defined by (9).

To demonstrate this, we follow the previous proof with the reference, in the end, to Theorem 2.1.

We know that, when using the multilevel T. Chan preconditioner, the number of outliers is $O(N(n) \sum_{k=1}^{p} \frac{1}{n_k})$ for any A_n generated by a continuous function f [19]. Therefore we can say that this preconditioning technique, unless not satisfactorily for large p, is the best that we may obtain when quasi-equimodular algebras are considered.

The last theorem apparently pertaines to many popular matrix algebra preconditioners. We have got now a rigorous proof that they can not be optimal, at least for the particular example of a multilevel Toeplitz matrix.

Note also that the basic results of Section 2 allow us to construct many other examples. In particular, there are Hermitian multilevel Toeplitz matrices (generated by a multivariable symbol) for which any Hermitian multilevel circulant-like preconditioner is not optimal.

To see this, take up the previous $f(x_1, \ldots, x_p)$ and consider the symbols

$$g_1 = \mathrm{Re}\, f(x_1, \ldots, x_p), \quad g_2 = \mathrm{Im}\, f(x_1, \ldots, x_p).$$

At least one of the sequences $I + A_n(g_1)$ or $I + A_n(g_2)$ can not have circulant-like optimal preconditioners. By contradiction, if both of them have optimal preconditioners $I + C_{n,1}$ and $I + C_{n,2}$, then the circulant-like preconditioner $I + C_{n,1} + \mathrm{i}C_{n,2}$ is optimal for $I + A_n(f)$ and this contradicts the main negative results of this section.

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