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BAND-TOEPLITZ PRECONDITIONED GMRES ITERATIONS FOR TIME-DEPENDENT PDES*

DANIELE BERTACCINI[1,⋆] and MICHAEL K. NG[2,⋆⋆]

[1] *Dipartimento di Matematica "Guido Castelnuovo", Università di Roma "La Sapienza", P.le Moro 2, 00185 Roma, Italy. email: bertaccini@mat.uniroma1.it*

[2] *Department of Mathematics, The University of Hong Kong, Pokfulam Road, Hong Kong. email: mng@maths.hku.hk*

Abstract.

Nonsymmetric linear systems of algebraic equations which are small rank perturbations of block band-Toeplitz matrices from discretization of time-dependent PDEs are considered. With a combination of analytical and experimental results, we examine the convergence characteristics of the GMRES method with circulant-like block preconditioning for solving these systems.

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1 Introduction.

The main aim of this work is to study the performance of a preconditioning methodology destined for use with iterative Krylov subspace techniques to compute the solution of the nonsymmetric linear systems arising from the numerical solution of systems of time-dependent partial differential equations (PDEs). In particular, some techniques to give a priori upper bounds for the number of preconditioned GMRES iterations are considered.

To introduce the problem, let us consider the following PDE

$$\frac{\partial u(x,t)}{\partial t} + \mathcal{L}u(x,t) = g(x,t), \quad x \in \hat{\Omega}, t \in [t_0, T], \tag{1.1}$$

where $\hat{\Omega}$ is the spatial domain, u is a vector containing the solution functions, $\mathcal{L}$ is the linear differential operator in space and g is the forcing term, with suitable initial and boundary conditions. Semidiscretizing (1.1) by using finite

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differences or finite elements, we have a system of ordinary differential equations

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = f(t, y(t)) := Jy(t) + g(t), \quad t_0 \le t \le T, \tag{1.2}$$

where $y(t), g(t)$: $\mathbb{R} \to \mathbb{R}^m$, $J \in \mathbb{R}^{m\times m}$, g is a smooth function and (1.2) is coupled with suitable conditions. Here, the Jacobian matrix J of (1.2) is assumed to be diagonalizable.

To approximate the solution of (1.1), and thus of (1.2), we consider a generalization of a linear multistep technique, i.e., linear multistep formulas but used in boundary value form (see, e.g., [1], and the references therein). Those methods approximate the solution of (1.2) by means of a discrete boundary value problem. The latter is obtained by using a k-step linear multistep formula of order p over a mesh that, for simplicity, can be supposed uniform, i.e., $t_j = t_0 + jh$ with $j = 0, \dots, s$ and $h = (T - t_0)/s$:

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \quad n = 0, \dots, s-k, \tag{1.3}$$

y_n is the discrete approximation to $y(t_n), f_n = f(t_n, y_n) \equiv Jy_n + g_n, g_n = g(t_n), n = 0, \dots, s$ and the values $y_0, \dots, y_{\nu-1}, y_{s-k+\nu+1}, \dots, y_s$ should be given. We observe that an initial value problem for (1.2) provides only the initial value y_0 or, e.g., a two-point boundary value problem provides the values y_0 and y_s. In general, the discrete problem based on (1.3) requires ν initial and $k - \nu$ final conditions. The other conditions can be supplied by coupling (1.3) with other schemes which lead to a set of difference equations independent of those in (1.3); see [2] for details. The discrete problem generated by the application to the problem (1.1) and thus (1.2) can be reduced to a linear system of algebraic equations. For example, if (1.1) is a continuous initial value problem with assigned initial conditions, thus such that $y_0 = \eta \in \mathbb{R}^m$ in is given, the discrete problem is then given by the following linear system

$$My = e_1 \otimes \eta + h(B \otimes I)g, \tag{1.4}$$

where

$$\begin{aligned} e_1 &= (1, 0, \dots, 0)^{\mathrm{T}} \in \mathbb{R}^{s+1}; \qquad y = (y_0, \dots, y_s)^{\mathrm{T}}, \\ g &= (g_0, \dots, g_s)^{\mathrm{T}} \in \mathbb{R}^{m(s+1)}, \qquad M = A \otimes I - hB \otimes J, \end{aligned} \tag{1.5}$$

and $A, B \in \mathbb{R}^{(s+1)\times(s+1)}$ are small rank perturbations of Toeplitz matrices that, in general, are nonsymmetric and nonnormal. For more details, see [2].

1.1 Block circulant and skew-circulant preconditioners.

In [2], the use of Krylov subspace methods with block-circulant preconditioners was proposed to solve (1.4). The block preconditioner considered is given by

$$P = \breve{A} \otimes I_m - h\breve{B} \otimes J, \tag{1.6}$$

where $\breve{A}, \breve{B}$ are suitable approximations of matrices A, B, respectively, while J is the Jacobian matrix or a suitable approximation $\hat{J}$. Two approximations for A, B are considered here. The first one is based on the P-circulant matrices introduced in [2]. It is defined as (1.6) where $\breve{A}$ and $\breve{B}$ are P-circulant matrices, or, for short, P-circulants, i.e., are circulant matrices whose entries of their first rows $\tilde{\alpha}_0, \ldots, \tilde{\alpha}_s$ and $\tilde{\beta}_0, \ldots, \tilde{\beta}_s$ are given by

$$\begin{aligned} \tilde{\alpha}_j &= \left(1 + \frac{j}{s+1}\right)\alpha_{j+\nu} + \frac{j}{s+1}\alpha_{j+\nu-(s+1)}, \quad j = 0, 1, \ldots, s, \\ \tilde{\beta}_j &= \left(1 + \frac{j}{s+1}\right)\beta_{j+\nu} + \frac{j}{s+1}\beta_{j+\nu-(s+1)}, \quad j = 0, 1, \ldots, s, \end{aligned}$$

respectively.

Besides that preconditioner, the generalized Strang preconditioner for (1.4) was considered in [2] and [7]. Unfortunately, such preconditioner can be ill-conditioned. For example, when the Jacobian matrix whose eigenvalues have real part being very small in modulus; see [2]. Thus, the second preconditioner we consider here was introduced in [4, 5] and is based on (1.6) where $\breve{A}, \breve{B}$ are skew-circulant approximations for A and B in (1.5), respectively. In particular, $\breve{A}$ is a skew-circulant matrix whose first row and column are given by $(\alpha_\nu \, \cdots \, \alpha_k \; 0 \cdots 0 - \alpha_0 \, \cdots \, -\alpha_{\nu-1})$ and $(\alpha_\nu \, \cdots \, \alpha_0 \; 0 \cdots 0 \; -\alpha_k \, \cdots \, -\alpha_{\nu+1})^{\mathrm{T}}$, respectively, and $\breve{B}$ is defined similarly. Note that the underlying approximations are the Strang-type skew-circulant preconditioners of A and B respectively; see [6].

In [2, 4, 5] we observed that the preconditioners (1.6) can be effective for several classes of problems. Preconditioners based on skew-circulant matrices for Hermitian and skew Hermitian Toeplitz problems can be found, e.g., in [6], and the references therein.

1.2 Rationale.

In a recent paper, we investigated the convergence rate of the conjugate gradient method for the underlying preconditioned systems with the normal equations approach; see [3]. In this paper, we examine the convergence properties of GMRES for the left preconditioned linear systems in (1.4) using the block preconditioners in (1.6). We stress that the arguments used in [3] cannot be extended to be used here for GMRES.

Our main concerns here are to understand the behavior of the preconditioned GMRES iterations for the underlying problem and the dependence on the step-size h associated with the time discretization. More precisely, for the considered problems, it is observed that the number of iterations required for convergence typically increases at most with $\mathrm{O}(\log s)$, where $h = \mathrm{O}(1/s)$. To this end, we consider the field of values, the pseudospectra and, in more detail, the eigenvalues and the eigenvectors of the underlying matrices. Moreover, for the problem considered we see that there is a tightly clustered set of eigenvalues contained in a region whose boundaries are independent of s, together with a small number of outlying eigenvalues that are independent of s.

In Section 2, two model problems are introduced in order to study the performances of the preconditioned GMRES iterative solver. In Section 3, the field of values, pseudospectra and eigenvalues of these preconditioned matrices are considered to give bounds for the number of iterations. However, for the last approach, the nonnormality of the matrices involved is also considered through the condition number of the matrices of the eigenvectors.

2 Model problems.

Before introducing the tools for convergence bounds, let us consider two simple model problems. We stress that, e.g., in [2] two-dimensional PDE examples are considered as well. In particular, the heat equation with constant and variable diffusion coefficient were used as model problems. However, we observed experimentally (see, e.g., [2]) the convergence behavior of GMRES which is very similar to that observed here.

Problem 1. Heat equation

Let us consider the heat equation

$$\begin{cases} \dfrac{\partial u}{\partial t} - c\dfrac{\partial^2 u}{\partial x^2} = 0, \\ u(0,t) = u(x_{\max},t) = 0, \quad 0 \leq t \leq 2\pi, \\ u(x,0) = x, \qquad\qquad\qquad 0 \leq x \leq \pi. \end{cases} \tag{2.1}$$

If we discretize the operator $\partial^2/\partial x^2$ in (2.1) with centered differences and stepsize $\delta x = \pi/(m+1), x_j = j\delta x$, the following system is obtained:

$$\begin{cases} y'(t) = T_m y(t), \quad 0 \leq t \leq 2\pi, \\ y(0) = \eta, \qquad\qquad \eta = (x_1 \cdots x_m)^{\mathrm{T}} \end{cases} \tag{2.2}$$

and the $m \times m$ Jacobian T_m is a symmetric tridiagonal Toeplitz matrix where its stencil is given by $(\delta x)^{-2}[1,-2,1]$. As can be easily observed, the Jacobian matrix has negative eigenvalues. A method based on the implicit midpoint rule of order two (see, e.g., [1]) is applied in the sequel to solve (2.2).

Problem 2. Hyperbolic equation of first order

Let us consider the wave equation of first order with periodic boundary conditions:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial u}{\partial x} = 0, \\ u(x,0) = g(x) = x(\pi - x), \quad 0 \leq x \leq \pi, \\ u(\pi,t) = u(0,t), \qquad\qquad 0 \leq t \leq 2\pi. \end{cases} \tag{2.3}$$

We discretize the partial derivative $\partial/\partial x$ with the central differences and step size $\Delta x = \pi/m, x_j = j\Delta x$. The following systems are obtained:

$$\begin{cases} y'(t) = L_m y(t), \quad t \in [0, 2\pi], \\ y(0) = \eta, \qquad\qquad \eta = (g(x_0) \cdots g(x_{m-1}))^{\mathrm{T}}, \end{cases} \tag{2.4}$$

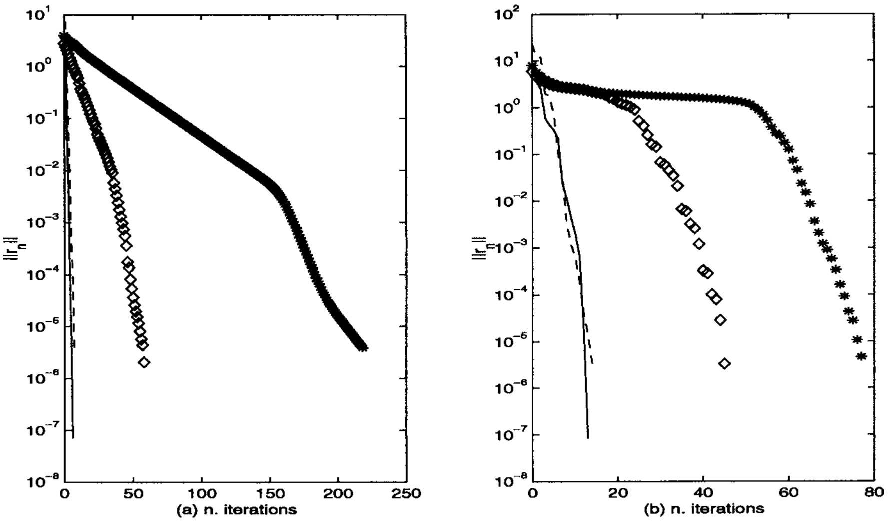

Figure 2.1: Convergence history. Continuous line: $s = 8$, $m = 10$; dashed line: $s = 32$, $m = 20$ for skew-circulant preconditioned iterations; diamond line: $s = 8$, $m = 10$, star line: $s = 32$, $m = 20$ without using preconditioner. (a) Problem 1 using the midpoint method; (b) Problem 2 using the fourth order generalized Adams-type method.

where the Jacobian matrix is $L_m = (2\Delta x)^{-1} H_m$ and H_m is a Toeplitz matrix where its stencil is given by $[1, 0, \ldots, 0, 1, \underline{0}, -1, 0, \ldots, 0, -1]$ (the underlined zero is on the main diagonal). As can be easily observed, the eigenvalues of the matrices $\{L_m\}$ are complex conjugate. A linear multistep formula in boundary form based on a fourth-order Adams formula with $k = 3$ is applied in the sequel to solve (2.4); see [4] for more details.

We present two sets of experimental results on convergence. All the computations described in this paper were performed using Matlab. The initial guess was identically zero, and the stopping criterion $\|r_j\|_2/\|r_0\|_2 < 10^{-6}$, where r_j is the residual vector at the jth iteration. Figure 2.1 shows the convergence histories of the nonpreconditioned iterations and skew-circulant preconditioned iterations for $s = 8$ and $s = 32$. These experiments clearly show that convergence of preconditioned iterations is essentially independent of the time discretization parameter.

3 Convergence bounds for GMRES.

In the following discussions, we consider the convergence process of the GMRES method in detail and determine some bounds on the number of iterations required for convergence of these preconditioned systems.

Let the preconditioned system under consideration be denoted now by $Kx = b$, and let the residual at the jth iteration r_j be given by $r_j = b - Kx_j$, where x_j is the j-step approximation of x. Recall that bounds for the GMRES method can

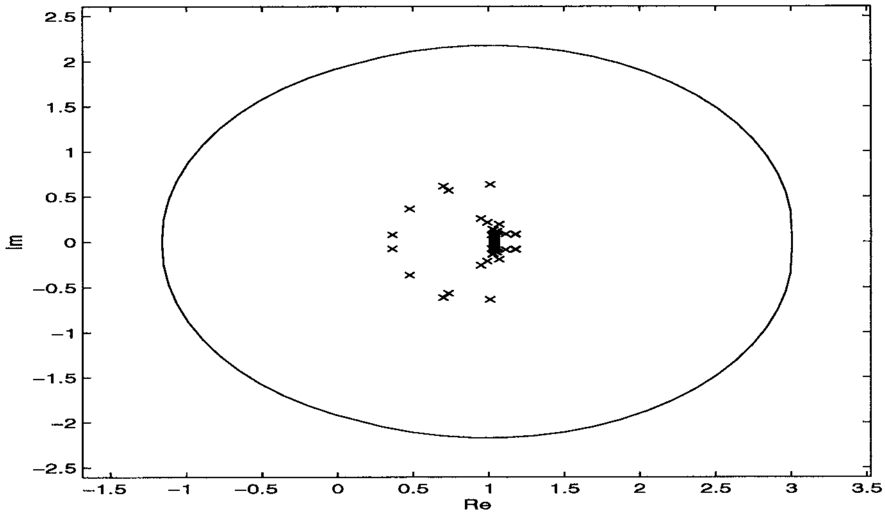

Figure 3.1: The field of values (its boundary is denoted by a solid line) of the preconditioned matrix for Problem 2 using a generalized Adam-type method with $s = 16$ and $m = 10$. The '$\times$' denotes the eigenvalues.

be determined by observing that (see, e.g., [11])

$$\|r_j\|_2 \leq \min_{p_j(0)=1} \|p_j(K)\|_2 \|r_0\|_2, \tag{3.1}$$

where the minimum is over all polynomials of degree j taking the value 1 at the origin. Thus, to give bounds for $\min \|p_j(K)\|$ in (3.1), and then to estimate the number of iterations for GMRES, we consider the *field of values*, the *pseudospectra* and, in more detail, the *eigenvalues/eigenvectors* approaches.

The approach based on the field of values can be very attractive since it is not influenced by the conditioning of the eigensystem and estimates can be obtained even for large matrices with a relatively moderate computational effort. Unfortunately, we have experienced that, even for our simple model problems, the field of values can severely overestimate the number of iterations required for convergence. However, the more severe limitation on the use of the field of values can be found in the fact that the related convex set can include the origin, even if the eigenvalues are strictly contained in the right half plane, see Figure 3.1, and thus the bound above cannot be used.

As suggested in [10], the pseudospectra of the matrix of the underlying linear system (1.4) can give some useful bounds for the number of GMRES iterations. For example, if the spectral condition number of the eigenvector matrix diagonalizing the preconditioned matrix K is huge, because of some nearly-defective eigenvalue of the Jacobian matrix J in (1.4), the use of pseudospectra can give very useful insights in the convergence analysis, see [10]. Unfortunately, an approach based on pseudospectra has to deal with three major difficulties in our case. The first one is the presence of several outliers, that must be considered. This can give misleading estimates because the outliers not too near to the

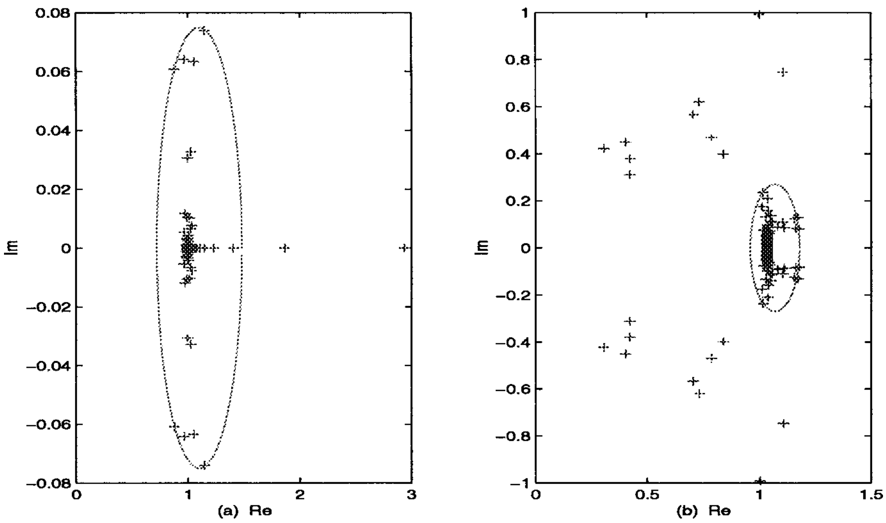

Figure 3.2: The spectra of the eigenvalues (denoted by '+') of the P-circulant preconditioned matrices for Problem 1 and Problem 2, $m = 10$, $s = 16$. The ellipse enclosing the cluster and some outliers is the boundary of the set Ω.

origin influence the convergence usually only introducing an initial delay without affecting the asymptotic behavior, see, e.g., [8]. The second difficulty is the cost for the pseudospectra computation, because the matrices considered here can be huge. Finally, the theoretical analysis of pseudospectra is difficult to perform, especially in the case of the underlying preconditioned matrices.

As observed in [2, 4, 7], the set of the eigenvalues of the matrix K can be mainly divided into two subsets: a set of clustered and a set of outliers. Figure 3.2 gives the spectra of the P-circulant preconditioned matrices for Problems 1 and 2. We can see from these figures that the preconditioned matrix has an eigenvalue distribution consisting of a set of clustered eigenvalues and a set of outliers.

Let us begin by restating a result that can be easily derived from (3.1). Assume that the $n \times n$ preconditioned matrix K is diagonalizable, i.e.,

$$K = V \Lambda V^{-1},$$

and let $\sigma(K)$ denote the set of eigenvalues of K. A popular bound on the convergence of the GMRES method is given by (see [11])

$$\|r_j\|_2 \le \kappa_2(V) \cdot \min_{p_j(0)=1} \max_{\lambda \in \sigma(K)} |p_j(\lambda)| \cdot \|r_0\|_2, \tag{3.2}$$

where $\kappa_2(V)$ is the spectral condition number of the matrix of the eigenvectors of K, V chosen to minimize $\kappa_2(V)$.

Let us consider the matrices K whose spectrum $\sigma(K)$ is clustered, as is the case of the underlying preconditioned matrices. It is natural to partition $\sigma(K)$ as follows

$$\sigma(K) = \sigma_c(K) \cup \sigma_0(K) \cup \sigma_1(K),$$

where $\sigma_c(K)$ denotes the clustered set of eigenvalues of K and $\sigma_0(K) \cup \sigma_1(K)$ denotes the set of the outliers. Here we assume that the clustered set $\sigma_c(K)$ of eigenvalues is contained in a convex set Ω.

Now, let us consider in more detail the sets

$$\sigma_0(K) = \{\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_{j_0}\} \quad \text{and} \quad \sigma_1(K) = \{\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_{j_1}\}$$

denoting two sets of j_0 and j_1 outliers, respectively. The sets σ_0 and σ_1 are defined such that, if $\hat{\lambda}_j \in \sigma_0(K)$, we have

$$1 < \left|1 - \frac{z}{\hat{\lambda}_j}\right| \le c_j, \quad \forall z \in \Omega,$$

while, for $\tilde{\lambda}_j \in \sigma_1(K)$,

$$0 < \left|1 - \frac{z}{\tilde{\lambda}_j}\right| < 1, \quad \forall z \in \Omega,$$

respectively. For example, in Figure 3.2, we observed experimentally that j_0 and j_1 are equal to 0 and 2 for the Problem 1, and j_0 and j_1 are equal to 12 and 8 for the Problem 2, respectively.

Under the above assumptions, we can state the following bound.

THEOREM 3.1. *The number of full GMRES iterations j needed to attain a tolerance ϵ on the relative residual in the 2-norm $\|r_j\|_2/\|r_0\|_2$ for the preconditioned linear system $Kx = b$, where K is diagonalizable, is bounded above by*

$$\min\left\{ j_0 + j_1 + \left\lceil \frac{\log(\epsilon) - \log(\kappa_2(V))}{\log(\rho)} - \sum_{\ell=1}^{j_0} \frac{\log(c_\ell)}{\log(\rho)} \right\rceil, n \right\}, \tag{3.3}$$

where

$$\rho^k = \frac{(a/d + \sqrt{(a/d)^2 - 1})^k + (a/d + \sqrt{(a/d)^2 - 1})^{-k}}{(c/d + \sqrt{(c/d)^2 - 1})^k + (c/d + \sqrt{(c/d)^2 - 1})^{-k}}, \tag{3.4}$$

and the set $\Omega \in \mathbb{C}^+$ is the ellipse with center c, focal distance d and major semi axis a.

PROOF. From (3.2), $\|r_j\|_2/\|r_0\|_2 \le \epsilon$ ($\ll 1$) is satisfied (in the exact arithmetic) if

$$\kappa_2(V) \cdot \min_{p_j(0)=1} \max_{\lambda \in \sigma(K)} |p_j(\lambda)| \le \epsilon, \tag{3.5}$$

where $\sigma(K)$ contains the set of eigenvalues of K and $p_j(z)$ is a j-degree polynomial. We have:

$$\min_{p_j(0)=1} \max_{z \in \sigma(K)} |p_j(z)| \le \max_{z \in \sigma(K)} |\hat{p}(z) \cdot q(z) \cdot \tilde{p}(z)|, \tag{3.6}$$

where

$$\hat{p}(z) = \left(1 - \frac{z}{\hat{\lambda}_1}\right) \cdots \left(1 - \frac{z}{\hat{\lambda}_{j_0}}\right), \qquad \tilde{p}(z) = \left(1 - \frac{z}{\tilde{\lambda}_1}\right) \cdots \left(1 - \frac{z}{\tilde{\lambda}_{j_1}}\right)$$

are the polynomials whose roots are the outlying eigenvalues in $\sigma_0 \cup \sigma_1$ and $q(z)$ is a polynomial of degree at most $j - j_0 - j_1 \geq 0$ such that $q(0) = 1$. Using the notations above, we have

$$|\hat{p}(z)| \leq \prod_{\ell=1}^{j_0} \left|1 - \frac{z}{\hat{\lambda}_\ell}\right| \leq \prod_{\ell=1}^{j_0} c_\ell$$

and

$$|\tilde{p}(z)| \leq \prod_{\ell=1}^{j_1} \left|1 - \frac{z}{\tilde{\lambda}_\ell}\right| \leq \prod_{\ell=1}^{j_1} 1 \leq 1, \quad \forall z \in \Omega.$$

Therefore,

$$\max_{z \in \sigma(K)} |\hat{p}(z) \cdot q(z) \cdot \tilde{p}(z)| \leq \left(\prod_{\ell=1}^{j_0} c_\ell\right) \max_{z \in \Omega} |q(z)|. \tag{3.7}$$

The polynomial $q(z)$ can be chosen to be the shifted and scaled complex Chebyshev polynomial $q(z) = C_k((c - z)/d)/C_k(c/d)$ which is small on the set containing $\sigma_c(K)$. Indeed, by using results on Chebyshev polynomials (see [11, Sections 6.11.2, 6.11.4]) we can derive the following bound

$$\begin{aligned} \max_{z \in \Omega} |q(z)| &= \frac{C_k(a/d)}{|C_k(c/d)|} \\ &= \frac{(a/d + \sqrt{(a/d)^2 - 1})^k + (a/d + \sqrt{(a/d)^2 - 1})^{-k}}{(c/d + \sqrt{(c/d)^2 - 1})^k + (c/d + \sqrt{(c/d)^2 - 1})^{-k}}. \end{aligned} \tag{3.8}$$

An upper bound on j now easily follows from (3.6), (3.7), (3.8) and by observing that, in exact arithmetics, GMRES converges in at most n iterations:

$$j - j_0 - j_1 = \left\lceil \frac{\log(\epsilon)}{\log(\rho)} - \frac{\log(\kappa_2(V))}{\log(\rho)} - \frac{\sum_{\ell=1}^{j_0} \log(c_\ell)}{\log(\rho)} \right\rceil$$

from which (3.3) follows. $\square$

We stress that

$$\rho \backsimeq \tilde{p} = \frac{a + \sqrt{a^2 - d^2}}{c + \sqrt{c^2 - d^2}}.$$

In particular, when the major axis is parallel to the imaginary axis, is centered in $(c, 0), c > 0$, and has length $2a$, while the minor axis $2b$, respectively, we have $a \geq b$ and

$$\tilde{\rho} = \frac{a + \sqrt{a^2 - |a^2 - b^2|}}{c + \sqrt{c^2 + |a^2 - b^2|}} = \frac{a + b}{c + \sqrt{c^2 + a^2 - b^2}},$$

and we use this expression to approximate ρ in the bound (3.3) in practice for our model problems.

According to Theorem 3.1, the outliers do not affect the asymptotic convergence rate of the GMRES method, but rather they introduce a latency effect of $j_0 + j_1$ iterations plus the term $\sum_{l=1}^{j_0} \log(c_l)/\log(\rho)$; see (3.3).

We stress that the condition number of V cannot be neglected in the above bound, otherwise the eigenvalues alone can give highly misleading information on the convergence process, see [9]. On the other hand, if V has a huge condition number (e.g., growing exponentially with the size of the matrix), the underlying bound is useless.

3.1 Eigenvector matrix.

Next we derive bounds on the condition number of the eigenvector matrix of the underlying preconditioned matrix, i.e.,

$$K = (\breve{A} \otimes I - h\breve{B} \otimes J)^{-1}(A \otimes I - hB \otimes J), \tag{3.9}$$

where $\breve{A}$ and $\breve{B}$ can be, e.g., P-circulant preconditioners or skew-circulant preconditioners for A and B, respectively, see Section 1.1.

THEOREM 3.2. *Assume that J is diagonalizable, i.e., $J = U\Sigma U^{-1}$. The condition number $\kappa_2(V)$ of the eigenvector matrix V of the preconditioned matrix K is bounded by*

$$\kappa_2(U) \cdot \max_{i=1,2,\ldots,m} \kappa_2(W_i),$$

where W_i is the eigenvector matrix of

$$\tilde{M}_i = (\breve{A} - h\mu_i\breve{B})^{-1}(A - h\mu_i B) \tag{3.10}$$

and μ_i is the ith *eigenvalue of $J, i = 1, 2, \ldots, m$. Moreover, the eigenvalues of the preconditioned matrix are given by*

$$1 + \sigma((\breve{A} - h\mu_i\breve{B})^{-1}((A - \breve{A}) - h\mu_i(B - \breve{B}))), \quad i = 1, 2, \ldots, m. \tag{3.11}$$

PROOF. We first note that

$$\begin{aligned}&(\breve{A} \otimes I - h\breve{B} \otimes J)^{-1}(A \otimes I - hB \otimes J)\\ &\quad = (I \otimes U)(\breve{A} \otimes I - h\breve{B} \otimes \Sigma)^{-1}(A \otimes I - hB \otimes \Sigma)(I \otimes U^{-1}).\end{aligned}$$

The matrix $(\breve{A} \otimes I - h\breve{B} \otimes \Sigma)^{-1}(A \otimes I - hB \otimes \Sigma)$ can be permuted to become the block-diagonal matrix $(I \otimes \breve{A} - h\Sigma \otimes \breve{B})^{-1}(I \otimes A - h\Sigma \otimes B)$ whose $(s+1) \times (s+1)$ diagonal blocks are given by $(\breve{A} - h\mu_1\breve{B})^{-1}(A - h\mu_1 B), \ldots,$ $(\breve{A} - h\mu_m\breve{B})^{-1}(A - h\mu_m B)$. Thus, we observe that the eigenvector matrix of $(I \otimes \breve{A} - h\Sigma \otimes \breve{B})^{-1}(I \otimes A - h\Sigma \otimes B)$ is also a block-diagonal matrix whose diagonal blocks are $W_1, \ldots, W_m$. Hence, the first result follows.

Table 3.1: The values of $\max_{i=1,\dots,m} \kappa_2(W_i)$ for the skew-circulant and P-circulant preconditioned matrices computed by a (preconditioned and rescaled) QR algorithm

		Problem 1		Problem 2	
m	s	Skew-circulant	P-circulant	Skew-circulant	P-circulant
10	8	6.7×10^1	1.0×10^1	2.7×10^1	1.1×10^1
	16	4.4×10^1	1.5×10^1	1.0×10^2	1.9×10^1
	32	4.5×10^1	2.8×10^1	3.0×10^2	2.1×10^1
	64	2.6×10^2	5.6×10^1	3.5×10^2	4.5×10^1
	128	1.3×10^2	1.2×10^2	2.3×10^2	7.2×10^1
	256	7.2×10^2	2.4×10^2	7.7×10^2	1.2×10^2
	512	1.9×10^2	5.1×10^2	6.4×10^2	2.0×10^2
	1024	1.3×10^3	1.0×10^3	9.6×10^2	3.4×10^2
20	8	4.4×10^1	1.0×10^1	2.4×10^1	1.1×10^1
	16	3.5×10^1	1.5×10^1	8.1×10^1	1.8×10^1
	32	7.5×10^2	2.8×10^1	3.4×10^2	2.9×10^1
	64	3.8×10^1	5.6×10^1	3.8×10^2	4.5×10^1
	128	5.9×10^1	1.2×10^2	6.1×10^2	7.2×10^1
	256	9.6×10^1	2.4×10^2	8.5×10^2	1.2×10^2
	512	1.9×10^2	5.1×10^2	9.1×10^2	2.0×10^2
	1024	1.3×10^3	1.1×10^3	1.7×10^3	3.4×10^2

Moreover, since the set of the eigenvalues of the preconditioned matrix are equal to the union of the sets of the eigenvalues of the matrices $\tilde{M}_i, i = 1, \dots, m$ (i.e., of the eigenvalues in each block) and

$$(\breve{A} - h\mu_i \breve{B})^{-1}(A - h\mu_i B) = I + (\breve{A} - h\mu_i \breve{B})^{-1}((A - \breve{A}) - h\mu_i(B - \breve{B})),$$

the formula (3.11) follows. □

The above results can give useful insights for many problems when the Jacobian matrix J is diagonalizable. For example, J is symmetric in Problem 1 and skew-symmetric in Problem 2, so U can be chosen orthogonal and therefore $\kappa_2(U)$ is equal to 1. However, if J is nonnormal and $\kappa_2(U)$ is very large, a bound based on pseudospectra should be used instead. In Table 3.1, we list $\max_{i=1,2,\dots,m} \kappa_2(W_i)$, where we recall that the size of the matrices W_i is $(s+1) \times (s+1)$. We see from Table 3.1, by using Theorem 3.2, that the condition number of the eigenvector matrix V of (3.9) grows as $\mathrm{O}(s)$ for the P-circulant preconditioners and faster for the skew-circulant. Thus, by using Theorem 3.1, it is worth noting that the number of the iteration grows at most with $\mathrm{O}(\log s)$ for the above mentioned examples. On the other hand, the condition number of the matrices of the eigenvectors for the nonpreconditioned matrix M in (1.4) can grow very fast with s, i.e., much faster than in the preconditioned case.

Table 3.2: Estimated and actual P-circulant preconditioned GMRES iterations for Problem 1

m	s	$\max_i \kappa_2(W_i)$	j_0	j_1	ρ	α	est-it	act-it
10	8	1.0×10^1	0	2	0.153	8.6	10.6	7
10	16	1.5×10^1	0	2	0.198	10.2	12.2	9
10	32	2.8×10^1	0	3	0.227	11.6	14.6	10
20	8	1.0×10^1	0	1	0.223	10.7	11.7	7
20	16	1.5×10^1	0	2	0.225	11.1	13.1	9
20	32	2.8×10^1	0	3	0.242	12.1	15.1	10

Table 3.3: Estimated and actual skew-circulant preconditioned GMRES iterations for Problem 1

m	s	$\max_i \kappa_2(W_i)$	j_0	j_1	ρ	α	est-it	act-it
10	8	6.7×10^1	0	3	0.0332	5.3	8.3	6
10	16	4.4×10^1	0	3	0.0537	6.0	9.0	6
10	32	4.5×10^1	0	3	0.0996	7.6	10.6	8
20	8	4.4×10^1	0	2	0.044	5.6	7.6	6
20	16	3.5×10^1	0	3	0.050	5.8	8.8	6
20	32	7.5×10^2	0	3	0.093	8.6	11.6	7

Table 3.4: Estimated and actual P-circulant preconditioned GMRES iterations for Problem 2

m	s	$\max_i \kappa_2(W_i)$	j_0	j_1	ρ	α	χ	est-it	act-it
10	8	1.1×10^1	6	6	0.188	9.7	2.97	24.7	16
10	16	1.9×10^1	6	4	0.214	10.9	2.28	23.2	16
10	32	2.1×10^1	6	4	0.194	10.3	2.33	22.6	16
20	8	1.1×10^1	12	2	0.229	11.0	6.67	31.7	22
20	16	1.9×10^1	16	4	0.178	9.7	4.97	34.7	21
20	32	2.9×10^1	12	2	0.224	11.5	4.90	30.4	19

3.2 Estimates of the number of iterations.

We have applied GMRES to solve the block (left) preconditioned system $Kx = b$ for the problems in Section 2 by using P-circulant and skew-circulant block preconditioners. Tables 3.2, 3.3, 3.4 and 3.5 show the comparisons between the estimate of the number of iterations (est-it) using the bound given in (3.3) and

Table 3.5: Estimated and actual skew-circulant preconditioned GMRES iterations for Problem 2

m	s	$\max_i \kappa_2(W_i)$	j_0	j_1	ρ	α	χ	est-it	act-it
10	8	2.8×10^1	8	4	0.595	6.1	1.90	20.0	13
10	16	1.0×10^2	10	4	0.158	10.0	0.58	24.6	11
10	32	3.1×10^2	10	4	0.058	6.9	0.12	21.2	9
20	8	2.4×10^1	20	16	0.064	6.2	2.87	45.1	18
20	16	8.1×10^1	20	8	0.027	5.1	2.87	36.0	13
20	32	3.4×10^2	20	8	0.115	9.1	1.40	38.5	14

the number of actual GMRES iterations (act-it) to attain a residual r_j such that $\|r_j\|_2/\|r_0\|_2 \leq 10^{-6}$. The columns labeled j_0 and j_1 are the cardinality of the sets $\sigma_0(K)$ and $\sigma_1(K)$, respectively. Recall that these sets contain the outlying eigenvalues. We note that, for Problem 1, we can choose the sets σ_c, σ_0 and σ_1 such that $\sigma_0(K)$ is empty. On the contrary, for Problem 2 some outliers are on the left-hand side of the clustered set of eigenvalues (cf. Figure 3.2) to avoid σ_c artificially stretched or including the origin of the complex plane. Otherwise, the bound (3.3) can be not sharp or not applicable at all.

The values of the factor ρ related to the underlying Ω (see Theorem 3.1) for the skew-circulant and for the Strang and modified Strang-type approximations are usually much smaller than those related to P-circulants. Recall that Ω is the convex set which contains the clustered eigenvalues. This implies that the spectra of the skew-circulant preconditioned are more clustered than those of the P-circulant preconditioned matrices. Therefore, the proposed bound can describe the performances for skew-circulant preconditioners only in a qualitative sense.

By putting the computed parameters $\max_i \kappa_2(W_i)$ as the upper bound of $\kappa_2(V), j_0, j_1$ and ρ in (3.3), we estimate the number of full GMRES iterations required for convergence for the underlying model problems.

In Tables 3.2–3.4, we also list upper bounds for the condition numbers of the eigenvector matrices V for K in (3.9). We can observe that the condition numbers of the eigenvector matrices for the P-circulant preconditioned matrices are usually lower than those related to the skew-circulants. This behavior is even more pronounced if the eigenvectors are computed without suitably preprocessing the preconditioned matrix K in (3.9). We experienced that the related eigenvectors are ill-conditioned, i.e. they have a condition number that can increase fast with s.

The preconditioned matrices related to the skew-circulant case (and similarly for Strang and others modified Strang-type approximations) have a (nondefective) eigenvalue 1 whose multiplicity is $\mathrm{O}(m(s-k))$ (k is the number of steps of the LMF formula (1.3)).

THEOREM 3.3. *Let the preconditioner as in* (1.6) *be based on skew-circulant approximations for* $\breve{A}, \breve{B}$. *Moreover, let* $\mu_1, \ldots, \mu_m$, *the eigenvalues of* J, *be such* *that* $\mathrm{Re}(\mu_r) \leq 0, r = 1, \ldots, m$. *Then, the eigenvalues of the preconditioned matrix are equal to* $(1, 0) \in \mathbb{C}^+$ *except for at most* $2mk$ *outliers.*

Proof. Apply [5, Theorem 10] with $\theta = \pi$. □

On the other side, P-circulant preconditioned matrices have a tight cluster of (complex conjugate) eigenvalues which are usually simple or with multiplicity at most r if, e.g., $\mu_i = 0, i = 1, \ldots, r \leq m$, centered in $1 + \hat{\delta}$, where $\hat{\delta}$ is a small real number (see [2] for details). In this case, we observed that the condition number of the matrix of the eigenvectors is usually lower than in the first case and depends linearly on s, even if the eigenvalue problem was not suitably preprocessed.

Finally, we found that the estimate for the number of iterations is quite in agreement with the behavior of the actual number of iterations. The discrepancy can be ascribed to the use of the worst-case style estimate (3.2) (see, e.g., the effect of the condition number of K on the bound mentioned above) and to the latency effect given by the outlying eigenvalues.

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